

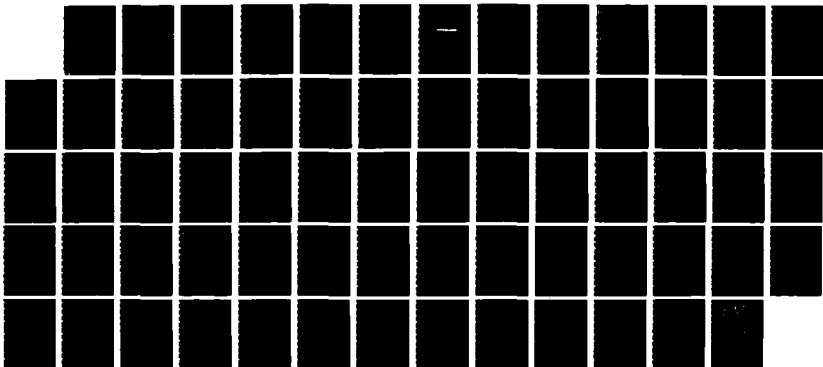
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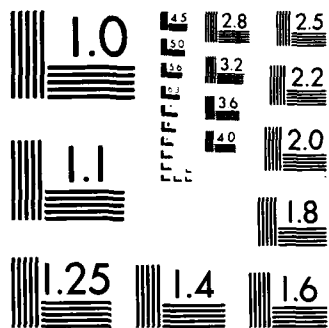
INTERNATIONAL CONFERENCE ON MICROSTRUCTOLOGY HELD IN
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DEPT OF MATERIALS SCIENCE AND ENGINE R T DEHOFF
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The conference was held as scheduled. The following objectives were addressed:

1. Examine the premise: The study of microstructure must be based upon concepts that admit no geometric assumptions.
2. Seek a consensus with respect to directions for development of the study of microstructures and microstructural behavior.

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Report on the

INTERNATIONAL CONFERENCE ON MICROSTRUCTOLOGY

May 7-9, 1986



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Report on the
INTERNATIONAL CONFERENCE ON MICROSTRUCTOLOGY

held at

Department of Materials Science and Engineering
University of Florida
Gainesville, FL 32611

May 7-9, 1986

The notion of presenting an International Conference on Microstructology, a meeting designed to develop in-depth discussion about how we conceive and perceive microstructures and their role in materials science, was originated by Dr. F. N. Rhines, Distinguished Service Professor Emeritus of the Department of Materials Science and Engineering at the University of Florida. It was unfortunate that Dr. Rhines passed away a few weeks before the meeting was held and could not be present to participate in these deliberations about a subject in which he had an abiding interest. By design, the meeting was to be small, with invited participants only and with the hope of attracting a world class list of participants. There were a total of eighteen presenters; seven of these came from Europe primarily to attend this meeting. The accompanying program illustrates the intent of the meeting; presentations were scheduled for from forty minutes to one hour so that there would be ample time for discussion. Two hour lunch breaks were included, again to foster leisurely discussion. It happened that the latter device was not implemented; so much discussion was generated in the morning sessions that they typically ran a full hour into the programmed lunch period.

A compilation of the abstracts for the presentations was prepared and presented to each participant, Appendix A. Additional copies were made available for the graduate students and faculty of the Department of Materials Science and Engineering who chose to sit in on the proceedings. Typically, their presence doubled the audience.

As is usual in meetings like this one, much of the interesting discussion about the topics of interest took place informally, outside of the meeting hall, at such opportunities as the welcoming reception on Tuesday, May 6, and the Conference barbeque on Thursday, May 8. Much of this discussion was animated and intense and, no doubt, later reflected in considerations during the day.

The stated objectives for the Conference were presented in the original proposal:

1. Examine the premise: The study of microstructure must be based upon concepts that admit no geometric assumptions.
2. Seek a consensus with respect to directions for development of the study of microstructures and microstructural behavior.

The extent to which these objectives were addressed and met has been assessed by circulating a Conference Summary and Questionnaire among the participants, Appendix B. The results of this survey are summarized in Appendix C.

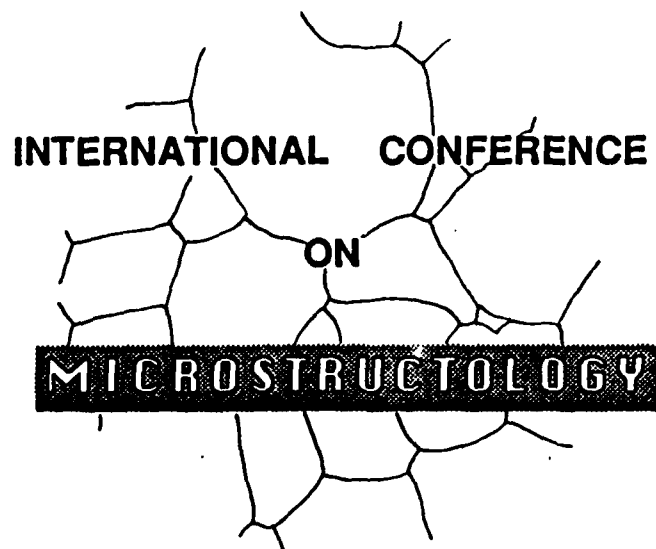
All who participated heartily agreed that the format of the conference, its subject matter, and its participants produced an intensive, and therefore very enjoyable, meeting of minds.

APPENDIX A

Program for the Conference

and

Copies of All Abstracts



Department of Materials Science & Engineering

**University of Florida
Gainesville, FL 32611**

May 7 To May 10

1986

PROGRAM

Wednesday, May 7

Morning Session

- | | |
|---------------|---|
| 9:00 - 9:10 | E. D. Verink, Jr.: Welcoming Remarks |
| 9:10 - 10:00 | F. N. Rhines and R. T. DeHoff: "Basis of Microstructology" |
| 10:00 - 10:20 | ✓ BREAK |
| 10:20 - 11:10 | ✓ H. E. Exner: "Shape: A Key Problem in Quantifying Microstructure" |
| 11:20 - 12:00 | ✓ H. Gundersen: "Quantitation of Microstructures without Geometric Assumptions" |
| 12:00 - 2:00 | LUNCH |

Afternoon Session

- | | |
|-------------|--|
| 2:00 - 2:50 | • Owen Richmond: "Space Tesselations for NonRandom Points and Particles" |
| 2:50 - 3:40 | ✓ • Brian Ralph: "Factors Controlling the Evolution of Grain Size During Grain Growth" |
| 3:40 - 4:00 | BREAK |
| 4:00 - 4:40 | • Hans Conrad: "Effect of an Electric Current during Recrystallization on the Size and Shape Distribution of the Resulting Grains" |
| 4:40 - 5:30 | General Discussion |

Thursday, May 8

Morning Session

- | | |
|---------------|---|
| 9:00 - 10:00 | • C. S. Smith: "Toward a Philosophy of Structural Change" |
| 10:00 - 10:20 | ✓ BREAK |
| 10:20 - 11:10 | • R. W. Cahn: "Antiphase Domain Boundaries, Grain Boundaries and the Ductility of Alloys" |
| 11:10 - 12:00 | • M. E. Glicksman: "Evolution of Microstructural Length Scales" |
| 12:00 - 2:00 | LUNCH |

Thursday, May 8

Afternoon Session

- | | |
|-------------|---|
| 2:00 - 2:50 | R. T. DeHoff: "Evolution of Porous Network Structures in Powder Processing" |
| 2:50 - 3:40 | • S. S. Chang: "Effect of Sintering Atmosphere on the Evolution of Pore Networks During Sintering of Copper Powder" |
| 3:40 - 4:00 | BREAK |
| 4:00 - 4:40 | • B. R. Patterson: "The Distribution of Grain Size and Faces per Grain During Grain Growth" |
| 4:40 - 5:30 | General Discussion |

Friday, May 9

Morning Session

- | | |
|---------------|---|
| 9:00 - 9:40 | ✓ • Gerhard Ondracek: "Microstructure-Property Correlations with Respect to Conductivity and Young's Modulus of Elasticity" |
| 9:40 - 10:20 | • Atul Gokhale and F. N. Rhines: "Effect of Grain Volume Distribution on the Plastic Response of Aluminum Polycrystals" |
| 10:20 - 10:40 | BREAK |
| 10:40 - 11:20 | • E. E. Underwood: "Analysis of Fracture Roughness Parameters" |
| 11:20 - 12:00 | • J. H. Steele: "Microstructure-Fracture Correlation - A Pandora's Box" |
| 12:00 - 2:00 | LUNCH |

Afternoon Session

- | | |
|-------------|---|
| 2:00 - 2:40 | • John C. Russ: "The Role of Image Analysis in Stereology" |
| 2:40 - 3:20 | / • J. P. Jernot: "Inexpensive System for Measurement of Stereological Parameters" |
| 3:20 - 3:40 | BREAK |
| 3:40 - 4:20 | ✓ • F. N. Rhines and Miguel Aballe: "Estimation of Growth Rates for Particles as Parts of a System" |
| 4:20 - 5:00 | R. T. DeHoff: "Toward a General Theory of Microstructural Evolution" |
| 5:00 - 5:30 | General Discussion |

Saturday, May 10

- | | |
|--------------|--|
| 9:30 - 12:00 | Informal and Optional Discussion Session |
| 12:00 | Conference Ends |

ABSTRACT

BASIS OF MICROSTRUCTOLOGY

By: F. N. Rhines

Microstructology is the science of the realistic and precise correlation of microstructure with the physical properties and processes of materials. Real microstructures of materials are always irregular in the sense that no two grains, or particles, in the structure are alike in size, shape or arrangement in space. Despite this irregularity, all of the parts fit together to form a continuous structure. Microstructology characterizes such structures by the exclusive use of the global parameters of geometry, some of which are drawn from the field of Stereology. No geometric assumptions of any kind are permitted. The relationships and mechanisms are deduced rather than postulated. These are all revealed as a product of structural characterization in the course of physical change.

BASIS OF MICROSTRUCTOLOGY

By: F. N. Rhines

Microstructology is the science of the statistically exact and fully realistic correlation of the microstructures of materials with their physical properties and processes. It seeks to make an exact science of the traditionally descriptive science of metallography.

There exists general agreement that the properties of materials and the physical processes that characterize materials are all critically dependent upon microstructure. It follows that the acquisition of an understanding of the behavior of materials requires a full knowledge of the real nature of microstructure and how it evolves. This is not the simple task that it might appear, because microstructures of materials are sophisticated in unsuspected ways. They are not actually difficult to comprehend, but they do have hidden characteristics that are not exposed by conventional means of dealing with geometric problems. Little heed has been paid, thus far, to rigor in the expression of microstructure in the formulation of relationships in physical metallurgy, with the result that this field has not progressed as it should. It is time to face the facts and to place the subject on a firm, realistic foundation. This is the mission of microstructology. It is a primary tenet of microstructology that no geometric assumption is admissible.

In approaching microstructure realistically it is necessary to admit two obvious, but disquieting, facts, namely: (1) that there are no exactly repeating patterns in the microstructures of materials and (2) that, despite this apparent disorganization, the parts of the structure fit together precisely to fill space. Far from being barriers to understanding, these two characteristics provide the keys to ultimate comprehension.

Although microstructures of materials usually display some typical feature by which they are recognized, such as being fine grained, coarse grained, lamellar, acicular, equi-axed or dendritic, none of these terms is truly definitive. When microstructure is examined critically, it is observed that no two of its parts are exactly alike in size, shape or spatial arrangement. This fact has seemed to the metallographer to present an obstacle to correlation with properties. He has sought to find something regular that he could measure and, in so doing, he has envisioned some kind of repetitious structure composed of units of average size, shape or average spacing of its parts. The result has, of course, been the exclusion from recognition of the essential diversity of structure. This has been ruinous to correlation with properties and processes, because without such diversity the complex changes in size and form which constitute such processes as grain growth, recrystallization, plastic deformation, sintering and phase transformations could not proceed. At any stage in any of these processes a broad range in changing particle size, shape and arrangement is required. Thus, a recognition of diversity in size, shape and arrangement in space is an absolute essential of microstructure-property correlation.

Microstructology responds specifically to the diversity of microstructure by the exclusive use of global parameters in measurement and the expression of structure. Since the global parameters measure the total of each geometric property in unit volume of the material, the difference from particle to particle does not affect the precision of the measurement. Each feature of the structure is thus measured in its natural dimension, which is to say that lineal feature is reported as a total length, surface feature as total area and spatial feature as total volume. This is very important, because only

in this way can the properties of size and shape be distinguished. The size of a grain, for example, cannot be expressed exactly in terms of a diameter, or of a cross-sectional area, because these parameters vary irregularly with shape. Assumptions of shape to compute volume from length, or area, are necessarily spurious for a variety of reasons, of which the diversity of shapes in microstructure is perhaps the most persuasive. Only the volume of the grain is independent of its shape and this provides the only exact measure of the size of a three-dimensional body. Thus, the dictum that no geometric assumption is admissible in microstructology excludes all but the natural parameters in the description of microstructure.

The fact that the parts of real microstructures of materials are all diversified does not, however, exclude the possibility that they can be classified with respect to their natural dimensions. The grains of an aggregate can be physically separated and sorted by volume, in order to describe a distribution. Indeed, other geometric features of the grains, such as surface area, edge length, number of facets, of edges and of corners can also be evaluated and classified. Such a description is global, as are the dimensional parameters. This provides statistical access to the dimensions of the individual particles in the aggregate, as well as to their topological shapes. In this way, the global parameters can provide both general and detailed information about microstructure.

Also of vital importance in the realistic representation of the microstructure of materials is the afore-mentioned second key characteristic, the continuity of structure. It is obvious that continuity of structure is necessary to the physical properties and processes, which are observed as characteristics of the whole material, not of its individual parts.

The properties of interest exist because the structure is continuous and space-filling and because the parts interact as a system to modify their individual characteristics. Tensile properties, for example, cannot be predicted from the critical resolved shear stress of the crystalline matter, because each grain and each particle in the aggregate is stressed differently, giving rise to a collective tensile property resulting from the interaction of all of the grains and particles in the system. Interaction is particularly evident in plastic deformation, where the response of each grain is contingent upon the shape changes of its many neighbors, both adjacent and distant. In grain growth and particle coarsening, no grain, or particle, can change its volume without a compensating change being distributed among its neighbors to maintain constant volume of the body of material. Hence, an expression of continuity is also an essential part of the correlation of structure with properties.

Continuity comes with mutual contact among the parts of the structure, each such contact existing as an interface, which may be a surface where two bodies meet, an edge where three bodies meet, or a corner where a meeting of four bodies occurs. The interfaces define the topological structure of the space-filling aggregate, as specified by the parameters: number and connectivity. Two-dimensional interface may exist in a number of separate parts, as in the case of the interfaces of particles embedded in a matrix. Topologically, the connectedness of this structure is zero and its number is the same as the number of particles. In the case of a polycrystalline aggregate, a single multiply-connected interface of grain boundary defines the system. It is characterized by its topological connectedness. Its parts, the individual grain facets, the grain edges and the grain corners, are described by the topological number of each. More complex structures may

be composed of several kinds of two-dimensional interface, existing partly, or wholly, as separate surfaces and perhaps also as one or more kinds of multiply-connected networks. In such case the system, as a whole, has a connectivity, but this may be broken down into connectivities of the different networks. The topological parameters are, of course, global.

A complete description of the microstructure of a material would be composed of many global parameter values corresponding to the topological parameters, the dimensional parameters, including the curvatures, and the distributive parameters. Such a system may be adequate to describe the structural function of a physical property, or process. Indeed, several examples of apparently complete descriptions have been found. But, it is evident that there are cases in which this system of parameters is not sufficient, showing that there remains need for the further development of the range of global geometric parameters. An example exists in the case of first stage sintering, which cannot be described completely with the present set of parameters.

The applications of microstructology, in addition to that of describing microstructure in a precise and realistic manner, include the study of the behavior of materials and the exact expression of structure-property and structure-process relationships. One of the most unexpected and dramatic products of using the global parameters in the investigation of physical processes has been the revelation of hitherto unknown characteristics which often clarify the mechanism of the process and always assist in its mathematical formulation. Consider an example. The metallurgical process that is called homogenization consists in heating a two-phased alloy in order to cause the lesser phase to dissolve in the major phase. It has been postulated that individual particles of the minor phase dissolve independently in the matrix, the average particle size decreasing until

solution is completed. Mechanisms based on this idea have fallen short of describing the process satisfactorily. When, however, the microstructure is characterized by its global parameters, in the course of homogenization, it is found that the average particle size remains constant, while the number of particles decreases until all are dissolved. The number of undissolved particles is proportional to the reciprocal of the time of heat treatment. These observations imply a much more sophisticated process than had been postulated. It suggests that the individual particles dissolve at different rates, that are proportional to the reciprocal of their sizes. The smaller particles dissolve faster, maintaining a fixed particle size distribution. It is significant that this process was not discovered by the conventional procedure of postulation and testing in the laboratory, but that microstructology led directly to the answer. This is probably because the postulator has a large number of possibilities to choose from, so that the likelihood of his success is small, whereas the characterization of microstructure leads directly to the only possible solution. The recommended procedure in the investigation of any structural process is to make no assumptions, but to characterize the microstructure as a function of progress. If the characterization is sufficiently comprehensive, the mechanism and rate of the process can be deduced.

An outstanding feature of the microstructology descriptions of processes that have been so analyzed thus far is that their mathematical expressions are not only exact, but they include only factors that are fully defined and are measurable. No curve fitting, or introduction of correction factors are encountered. Without going through their derivation, two examples will be cited. The tensile force exercised by a mass of sintering metal powder as it contracts is called the sintering force (F/a). This arises from the surface tension (γ) acting upon the curved surface of the porous mass.

When the microstructure is characterized with respect to its total surface area (S_v), its total surface curvature (M_v) and the volume fraction of its porosity (V_v) it is found that:

$$F/a = \gamma M_v V_v / S_v$$

This is a precise relationship which has been used extensively for the accurate measurement of the surface tension of solids. It involves no approximations. It has the characteristics of a relationship of exact science.

A final example displays the additional synergism of the discovery of a new principle in the course of the analysis of the process. The case in question is steady state grain growth in a pure metal. The grain size is expressed as the grain volume and the average grain size is one divided by the number of grains in unit volume ($1/N_v$). This is found to vary directly with the time of growth at elevated temperature. A comparison of the global parameters revealed that the ratio: $M_v S_v / N_v$ is a constant throughout grain growth at fixed temperature. Subsequently, it was found that the standard deviation of the grain volume distribution is also constant during isothermal grain growth and that its numerical value is nearly the same as that of the ratio $M_v S_v / N_v$. When a rate equation was derived upon the basis that surface tension is the driving force for growth and grain boundary mobility the physical mechanism, it turned out that the principal structural factor is the afore-mentioned global parameter constant:

$$\left(\frac{1}{N_v}\right)_t - \left(\frac{1}{N_v}\right)_0 = \frac{M_v}{N_v} \frac{\gamma M_v S_v}{N_v} t$$

where M_v/N_v is the mobility of grain boundary in a net having N_v grains. Again, the equation contains only known and evaluable factors and has the form of a natural law of science. Microstructology is thus capable of creating an exact science of metallography.

Quantifying Microstructure

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Institut für Werkstoffwissenschaften, Stuttgart,
FR Germany

The quantitative assessment of the shape of microstructural features poses a number of problems most of which are not solved in general terms. A large number of shape parameters have been proposed in the literature some of which are usually easily accessible from simple measurements on planar cross sections, while some are based upon complex mathematical concepts like mathematical morphology, Fourier coefficients or fractal dimensions. Most of these parameters have severe deficiencies - lack of sensitivity, size dependence, ambiguous or undefined interpretation. Only a few of these parameters lend themselves to describing average shape and none describe aspects of shape simultaneously. Present concepts and their problems are reviewed and a pragmatic approach is suggested for quantifying various aspects of planar shape. This approach can be extended to describe three-dimensional shape if 3-D data (from serial sectioning or stereoscopic measurements) are available. Quantitative assessment of 3-D shape from planar sections is only possible for some of the most regular shapes while a global parameter for complicated and mixed shapes has not been found and is not in sight.

Concise modelling of mechanisms of processes which form and change the microstructure requires adequate descriptors for shape changes. Present analytical models for important processes like solidification, coarsening or sintering are usually based on structural units with simple regular shapes which, as a rule, are hardly in agreement with real structures. More realistic models apply shape independent global parameters. Successful approaches assume time independent but unspecified shape; shrinkage during viscous sintering is discussed as an example. Shape changes of microstructural features are usually described phenomenologically or by convenient planar shape descriptors on an empirical basis. Feasible alternatives to this "fingerprinting" are not available.

Only a few attempts have been made to assess the effect of shape on properties of materials. Empirical correlation with quantitative interpretation of the results rather than stringent modelling prevails.

Numerical modelling is sometimes useful to prove whether simplifying assumptions are adequate or if a detailed description of local shape variations may be needed to understand the behaviour of a particular material during an individual processing step or under a given set of conditions in application.

Factors controlling the evolution of grain size
during grain growth.

Brian Ralph and Valerie Randle
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University College, Cardiff, U.K.

Abstract

A material given a post recrystallisation anneal tends to develop a larger grain size. The driving force for this process is the reduction in grain boundary area (and therefore energy of the system) and the process itself may take a number of forms involving the uniform displacement of the whole grain size distribution to larger sizes (normal growth) or, at some stage in the process, the selection of particular size classes which grow at the expense of others (anomalous, or abnormal growth (also often termed secondary recrystallisation)).

Grain growth involves the migration of grain boundaries and this migration process may be controlled or selected by a number of factors. The presence of strong recrystallisation textures may lead to the production of grain misorientations where the boundaries have different mobilities. Likewise it is possible for the thermomechanical processing to lead to some grains having a particular initial size advantage over the grains which surround them. The presence of solute atoms tends to slow down the process of grain growth whilst particles/precipitates may interact with the migrating boundaries in such a way that the migration process is impeded or halted (by pinning).

There are several ways of assessing the effects that particles have on the grain growth process, which are considered in this presentation. Basically a "two-pronged" approach is adopted where the evolution of the grain size distribution is followed on the one hand, whilst, on the other, a detailed investigation of the interactions between particles and boundaries is also investigated as a means of assessing the balance of driving force versus restraint due to the particles. An attempt is made to interrelate the more macroscopic with the microscopic approach. Essentially the first approach considers the behaviour of the assemblage of grains and particles whilst the latter looks at specific interaction which takes into account factors such as the specific geometry of single boundaries.

In the first part of this investigation, which involves the behaviour of both a model dispersion-strengthened alloy and a commercial nickel-base superalloy, considerable thought has been given to the means of assessing the evolution of grain size distributions. A number of methods have been used which aim to give grain size distributions which may be compared with theory and also which show how the grain growth process proceeds. These methods have compared the conventional intercept approach with measurements of parameters such as Feret and equivalent circle diameters and have also been used to evaluate both the evolving two dimensional and three dimensional grain size distributions. It has been found possible to make clear distinctions between grain growth by various processes using this overall approach.

A detailed investigation has also been made of the interactions between specific particles and migrating grain boundaries using the techniques available on a modern analytical electron microscope. Interactions between both incoherent particles and coherent precipitates have been followed. In both cases this has involved looking at the local geometry of the grain boundary plane in the neighbourhood of the particle (to measure driving pressures) and the local boundary crystallography. Particle parameters, such as size distribution and volume fraction, in the matrix and in the grain boundary region have also been measured.

With incoherent particles which are stable the pinning forces are found to vary with the local grain boundary geometry such that low angle and special (near CSL) boundaries are more strongly pinned. As has been noted by many previous workers, where some of the particles are unstable with respect to dissolution or coarsening in grain boundaries, a tendency to the selective migration of some boundaries is noted leading to abnormal grain growth.

Coherent particles are found to be associated with much stronger pinning (as has been suggested in a number of recent modelling studies). The migrating grain boundary has the possibility of "cutting" through the particle (where the matrix/particle orientation relationship is maintained). This configuration is encountered relatively rarely whilst an attempt by the boundary to "by pass" particles is the much more common case. In the "by pass" process the particle is extensively modified by the migrating boundary and often the pinning of the boundary is found to be complete. This latter process leads to a major disruption of the microstructure in the local region of the boundary, which will be discussed.

A particularly interesting subset of the results from the study of the coherent particle/grain boundary interaction results from the measurements of the local grain boundary crystallographic parameters. It was noted in this case that long term annealing treatments frequently lead to no grain

growth so that the grain boundary area remained unchanged. However, what are in effect measurements of local texture have suggested an alternative means by which the energy of the system has been reduced. This has involved changes in the crystallography of grain boundaries to favour a higher percentage of them having lower energy configurations; in the particular case considered here there was found to be a three fold increase in the percentage of special (near CSL) grain boundaries. This should be contrasted with the case for the same alloy annealed at temperatures above the solvus for these coherent boundaries where normal grain growth was exhibited.

EFFECT OF AN ELECTRIC CURRENT DURING RECRYSTALLIZATION ON THE
SIZE AND SHAPE DISTRIBUTION OF THE RESULTING GRAINS

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It has been found by the author and his coworkers that the application of high density ($\sim 10^5$ A/cm²) d.c. current pulses (~ 100 μ s, at 2HZ) during the annealing of Cu enhanced the rates of recovery, recrystallization and grain growth. Moreover, there occurred such changes in microstructure as a finer recrystallized grain size, a reduction in twinning frequency and an increase in the roughness of the grain boundaries. An analysis of the kinetics for recrystallization suggested that the influence of the current was primarily on the pre-exponential factor of the Arrhenius rate equation.

In the case of Ti, the current pulsing retarded the rate of grain growth and sharpened the grain size distribution curve. The retarding effect of the current again appeared to be on the pre-exponential factor in the rate equation.

EFFECT OF COLD WORK ON THE GRAIN SIZE DISTRIBUTION IN TITANIUM

Hans Conrad
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Raleigh, N. C. 27695-7907

ABSTRACT

The grain size distribution in Ti recrystallized following 93% R.A. by swaging was determined by the linear intercept, planimetric and serial sectioning methods. The three size distributions were all log-normal. There existed an intrinsic spatial distribution of grain sizes, for which the mean values of the chord length $\bar{l}$; grain area $\bar{A}$ and grain volume $\bar{v}$ were related by

$$\bar{l} = \alpha(\bar{A})^{1/2}, \bar{l} = \beta(\bar{V})^{1/3} \text{ and } \bar{A} = \gamma(\bar{V})^{2/3}$$

where α , β and γ are approximately unity. Serial sectioning revealed that the number of faces, vertices and edges of the polyhedral grains increased with increase in grain size, and the larger the grain size the more nearly isotropic it became.

A decrease in the amount of cold work (94 to 22% R.A.) prior to annealing resulted in an increase in the standard deviation of the grain volume distribution $\ln \sigma_v$ deduced from one-dimensional linear intercept measurements. The increase in $\ln \sigma_v$ with decrease in amount of cold work in the swaged Ti is in good accord with that reported by Rhines and Patterson following uniaxial deformation of Al. The reason for the increase in $\ln \sigma_v$ with decreased cold work is not clear. The observed increased rate of grain growth with reduction in cold work can be understood in terms of the larger number of three-edged grain faces with the greater spread in the recrystallized grain volume distribution.

Toward a philosophy of structural change

The many branches of science are currently converging into a study of the relationship between the structures of matter and time and the structure of human thought. Philosophers saw that the properties of things in some way depended on their inner structure at least as early as the 6th century B.C. Long before this, however, artists and artisans had empirically discovered many of the principles underlying the aggregation of units and the generation of boundaries between regions differing in the density, orientation and/or shape of their parts. Wall mosaics composed in about 4500 B.C. at Uruk developed crystallographic anisotropy from the placing of circular parts. The geometric mosaic tiling of the Islamic mosque and Celtic patterns as in the Lindisfarne Gospels, which appear superficially similar, are profoundly different in the way they exploit hierarchical relationships.

An artist exploits the one-, two-, and three-dimensional nature of marks left by movements of pen, brush or graver to confer important qualitative differences on the nature of the finished work. Various distinctive forms of brush stroke are used in Chinese landscape paintings to generate and distinguish regions on the basis of substructural differences quite analogous to the molecular-structural distinctions underlying the differences between chemical phases. The recognition of boundaries in a painting as a function of the scale of perception and comparison in the human eye is remarkably similar to the formation of boundaries in a two-phase liquid system at the critical point and to spinodal separation within a the crystal lattice of a solid solution.

All discovery, perception and understanding of structure becomes at some stage a matter of the identification of the boundaries between xenomorphs and their environment --- but how thick and how complex is the boundary? How long does it take to establish differences between "inside" and "outside"? On what scale does microscopic granularity merge into macroscopic uniformity? The whole character of burgeoning mathematical science for almost two centuries has prevented attention to such questions. Atomism for good reason became triumphant in the late 17th century, but in the 20th century we are returning to an approach that has much in common with the qualitative corpuscular view that, under Aristotle's influence, was by far the most common in the middle ages.

The last of the corpuscularians, strongly influenced by René Descartes (1644), was Emanuel Swedenborg whose Principia rerum Naturalium (1734) contains very astute intuitive models of quantized interactions with scale-dependent alternation of structural degrees of freedom. For two centuries thereafter, however, the immense utility of new mathematical approaches using empirically determined constants had the effect of precluding a profound concern with real structures, and such advances as

occurred were observational. The atom is a fine basis for chemical arithmetic -- but it works only if the majority of compounds (which are non-stoichiometric) are ignored. Understanding in principle is a major block in the road to understanding. Infinitesimal calculus is fine for gross planetary trajectories or the idealised elasticity of solids. Euclidean plane-faced polyhedra are also useful in an empirical sort of way, but none of these depend on the actual substructure of matter. Despite the excellent beginning with the experimental studies of properties such as hardness, plasticity, and fracture by the Dutch physicist Pieter Musschenbroek in the 1720's, such topics were excluded from main-line respectable physics for almost two centuries. At present, however, both quantum theory and condensed matter physics are exploring the true hierarchy of stability and change in material structure. Time generates an enormous diversity of local regions the internal structure of which determines their continuing response to environmental fluctuation by microscopic shear or diffusion in a manner grossly computable as structural inertia within Clarence Zener's acoustic spectrum,

The advantages and disadvantages of the different ways of viewing crystal form will be discussed, and an account given of a recently rediscovered paper published by a Dominican priest named Truchet in 1704. In this, combinatorial principles are developed on the basis on tile orientations and it is shown how to produce diagrams of connection, disconnection, and enclosure on virtually any scale and with any degree of complexity and gross symmetry. Eighteenth-century decorative art used the scheme to some extent, but the principles were ignored by mathematicians and scientists.

23 February 1986

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ANTIPHASE DOMAIN BOUNDARIES, GRAIN BOUNDARIES AND THE DUCTILITY OF ALLOYS

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(Cambridge University)

The Hall-Petch Law relating grain size to flow stress of metals and alloys is the subject of scores of papers every year, but the relation of grain size to the ductility (tensile elongation) of polycrystals has been only patchily examined - except in connection with the special case of superplastic behavior, where the ductility is linked to the length of the diffusion path between different boundaries of the same grain.

Armstrong has recently proposed a Hall-Petch type relation between tensile ductility and mean grain size for several metals deformed by dislocation flow. Apart from this, even normally brittle alloys like NiAl and Ni₃Al can show considerable ductility if the grain size is well below 20 μm . Some alloys, e.g. alpha brass, behave in a contrary way, in that large grains confer better ductility. Some implications of these observations will be outlined.

However, recent experiments by a Japanese group in Sendai and by the author on ordered polycrystalline Ni₃Al and (Ni₃Al + Fe) alloys (collectively, " γ' ") have shown clearly that in these inherently brittle, ordered materials, another microstructural feature has a more important effect on ductility. This is the array of antiphase domains (APD's) sometimes found in ordered alloys. An extensive range of observation will be marshalled to prove that a microstructure of fine antiphase domains confers good ductility on γ'

phases, irrespective of grain size. It seems that APD boundaries can hold up or at least brake many dislocations, thus reducing the cumulative stress exerted by dislocation pile-ups on grain boundaries. APD's are not, it seems, potential fracture sites in themselves.

$\text{Ni}_{3+x}\text{Al}_{-x}$ has the very unusual property that the temperature T_0 (at which ordered γ' and disordered γ of the same composition have the same free energy) can be either above or below the freezing temperature, T_f , according to the non-stoichiometry parameter, x . T_0 is a "metastable ordering temperature". If $T_0 > T_f$, no or few APD's can apparently form, and the alloy is brittle. If $T_0 < T_f$, the alloy freezes in disordered form and then orders on further cooling, forming copious APD's as it does so. Such APD - containing alloys are ductile to a variable extent which seems to depend directly on mean APD size. The evidence will be presented in detail.

This finding marks several issues for microstructural study: (1) What is the functional relationship between tensile ductility and mean APD size, for constant grain size? (2) How do dislocations behave as they cross APD boundaries? (3) Can any way be found of injecting APD's into alloys for which $T_0 > T_f$ - e.g., by grain growth, recrystallization or conceivably by ultrafast solidification? The ideas behind this question will be explained.

A more general question would also benefit from systematic examination: How far is it justifiable to relate ductility merely to the mean grain or APD size, and how far is it determined by the largest grains or domains present - by loose analogy with the role of the largest cracks in brittle fracture statistics? (Local variations of APD size could be achieved by localized transient heating of a coarse-grained alloy). Such questions are apposite for rigorous stereological investigation.

EVOLUTION OF MICROSTRUCTURAL LENGTH SCALES

by

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Abstract of a presentation for the International Conference
on Microstructology, University of Florida, Gainesville, Florida,
May 7-9, 1986

ABSTRACT

When a pure supercooled melt is partially solidified, it will produce a fine solid microstructure embedded in a continuous liquid phase. The volume fraction of solid produced is determined by the initial undercooling and can be kept constant by imposing an external adiabatic constraint on the two-phase mixture. After the nucleation and growth of the solid phase, the mean temperature of the solid-liquid mixture will be depressed slightly below that of the bulk melting point of the material by an amount $\langle \Delta T \rangle$. This temperature depression is a capillary effect arising from the presence of highly curved solid/liquid interfaces which form the mixture's microstructure. The well-known Gibbs-Thomson equation states that the local equilibrium temperature is depressed by an amount, ΔT , which is proportional to the local total curvature of the interface. Therefore, the mean undercooling of the two-phase mixture, $\langle \Delta T \rangle$, when measured on a size scale much larger than that of the microstructure, reflects an average curvature of the microstructure.

The equilibrium temperature at a convex solid-liquid interface will be relatively lower than that near a flatter region. Heat will diffuse toward these cooler regions, causing sharply curved areas in the microstructure to re-melt and blunt, while flatter regions tend to grow. This microstructural coarsening is analogous to Ostwald ripening among isolated domains, with the statistical distribution of length scales in the microstructure corresponding to the size distribution of ripening particles. Theoretical treatments of Ostwald ripening kinetics indicate that the average curvature of the ensemble of particles decays as $\text{time}^{-1/3}$, and that the associated rate constant increases with increasing volume of second-phase particles because of the reduced interparticle diffusion distances. Similar qualitative effects are expected during diffusion-controlled microstructural coarsening in complex partially solidified systems.

Experiments have been performed on model systems, including succinonitrile (SCN), ice/water, and ethylene carbonate (ETC). Materials were either purified by zone refining and/or multiple distillation, and sealed under vacuum in glass ampules containing reentrant thermometer wells (See Fig. 1a). The mean temperature of the two-phase mixture is measured with a 50-ohm wire-wound platinum resistor, which has been calibrated against a standard platinum resistance thermometer. The platinum resistor is placed near the bottom of the thermometer well within the solid-liquid system. The thermometer resistance is measured with a resolution of 10^{-5} ohm and negligible zero-drift. Output signals are analysed with a microcomputer which converts the measured resistance to a temperature value using the IPTS-68 temperature scale. The resulting temperature resolution is 5×10^{-5} K, at approximately 300 K.

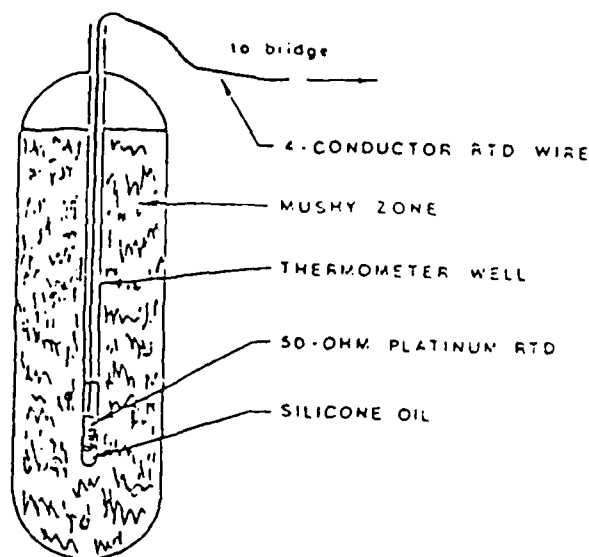
Temperature data are obtained by first heating the ampule until the material is completely melted, and then transferring the molten sample to a bath which is maintained at the desired initial supercooled temperature. When the temperature of the material in the ampule stabilizes, the solid phase is nucleated. The ampule is immediately transferred to a second constant-temperature bath set about 2 mK below the equilibrium melting point of the material. This bath maintains a constant volume fraction of solid in the two-phase mixture by preventing heat flow to or from the ampule. The microcomputer records the mean temperature in the ampule at equal intervals on a $(\text{time})^{-1/3}$ scale, starting at 125 seconds after nucleation of the solid phase and continuing to about 40,000 seconds. Signal averaging techniques are used to determine the average temperature at the end of each time interval. These data are then stored on disk for later analysis and plotting. Figure 1b shows a schematic of the overall system.

Plots of temperature-time data indicate that the mean undercooling $\langle \Delta T \rangle$ decays as $(\text{time})^{-1/3}$. This behavior is verified for SCN which develops a highly branched dendritic microstructure, and for ETC (Fig. 2), which solidifies from the melt with a needle-like morphology, and for ice/water which forms plate-like hexagonal dendrites reminiscent of snow flakes. The slope of the linear range of data on these plots of $\langle \Delta T \rangle$ vs. $(\text{time})^{-1/3}$ strongly suggests a diffusive coarsening rate constant. This slope is observed to increase as the volume fraction of solid in the microstructure increased (Cf. Figs. 3a and 3b). These observations are in qualitative agreement with the theoretical treatment of microstructural coarsening as a statistical ripening phenomenon.

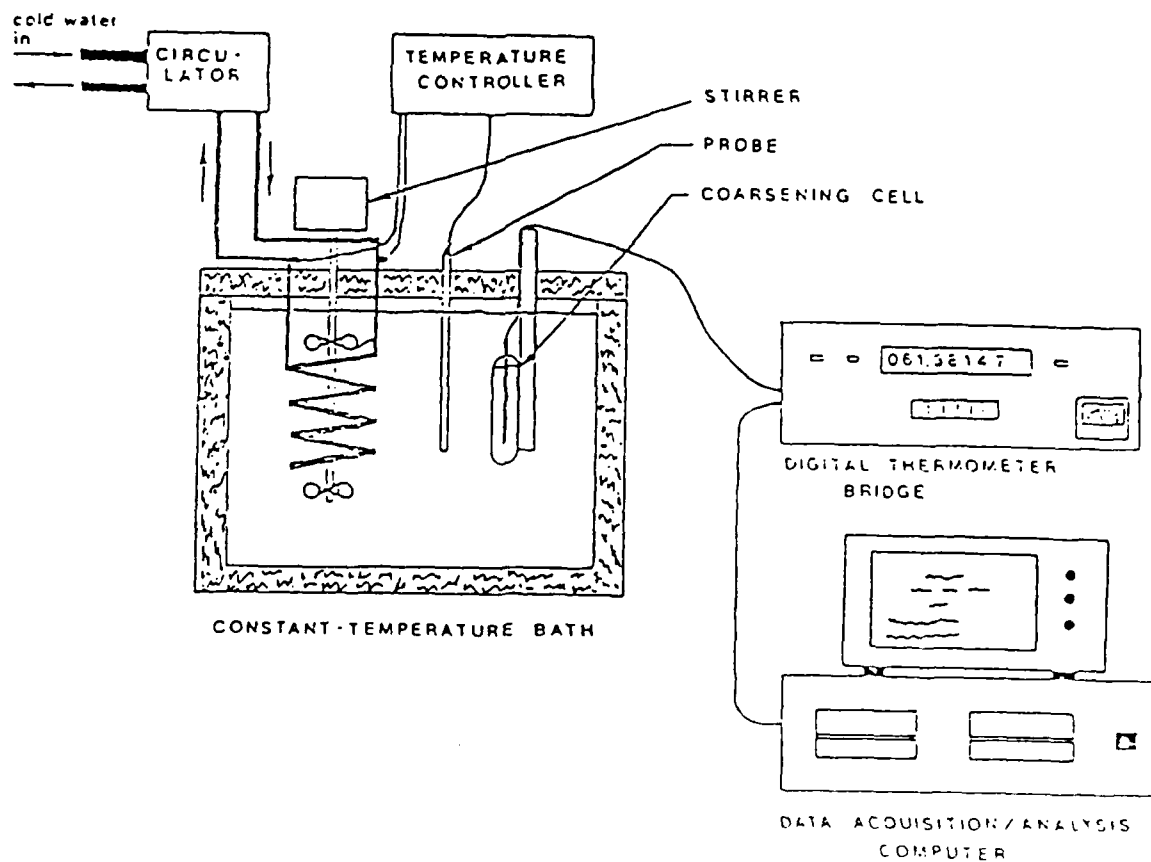
The implications of these observations will be discussed along with pertinent theories of coarsening in solid-liquid mixtures, and fundamental connections of important lengthscales, timescales, and thermophysical properties will be underscored.

ACKNOWLEDGEMENT

The authors gratefully acknowledge the support provided by the National Science Foundation, Division of Materials Research under Grant DMR 83-08052.



(a)



(b)

FIGURE 1: (a) Diagram of the glass ampule used in the coarsening experiments, showing details of the thermometer structure.
 (b) Schematic drawing of the experimental apparatus used to study coarsening kinetics in-situ.

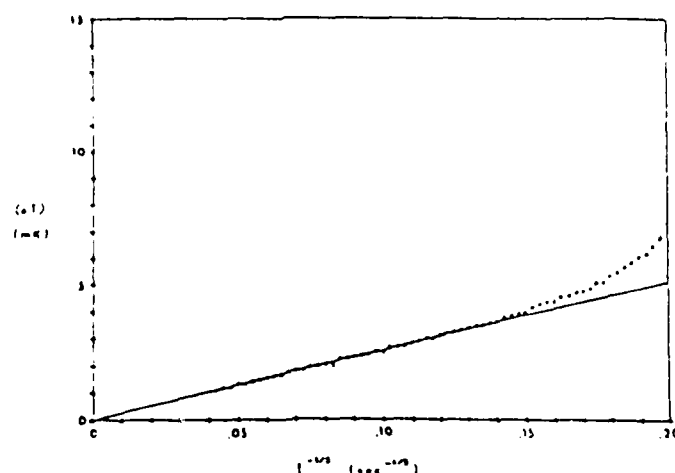
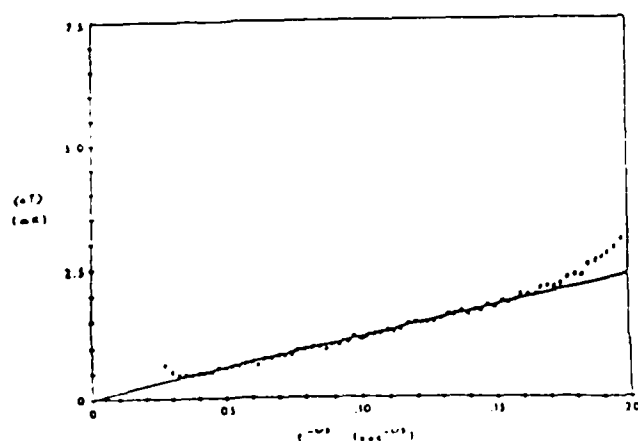
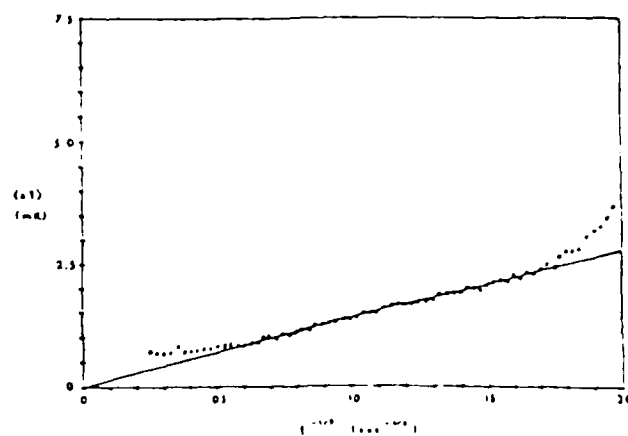


FIGURE 2: Coarsening data for ETC. The solid-liquid microstructure contains about 7% solid, with a calculated rate constant of $25.6 \pm 0.4 \text{ mK-sec}^{1/3}$.



(a)



(b)

FIGURE 3: Coarsening data for SCN

- (a) Microstructure containing 11% solid. The slope of the straight line indicates a rate constant of $11.9 \pm 0.4 \text{ mK-sec}^{1/3}$.
- (b) Similar data for a microstructure containing 16% solid, with a corresponding rate constant of $13.9 \pm 0.4 \text{ mK-sec}^{1/3}$.

EVOLUTION OF POROUS NETWORK STRUCTURES IN POWDER PROCESSING

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Powder processing provides a useful vehicle for the contemplation of network structures and how they evolve. The volume fraction of porosity may vary from over 90% to zero. The topology of the structure may be systematically varied by design of the powder stack. The path of microstructural change traversed may be significantly altered by processing conditions.

There are kinds of networks that develop in other microstructural contexts that are clearly geometrically very different from the porous structures that develop in powder processing: lamellar and other eutectics; some spinodals; grain edges. Nonetheless, porous structures arising in powder processing provide a comprehensive range of geometric conditions which may be sampled in a reasonably systematic way.

This presentation reviews paths of microstructural change observed in powder processing, including information about both the metric and topological properties of the pore network. Emphasis is on the powder, stacking, and processing variables that influence the path of evolution. The results will be used to focus upon two points for discussion:

1. The number of degrees of freedom that such structures may possess in their geometric properties; structures have been encountered in which, for a given volume fraction, the surface area and total curvature are identical, yet the structures are topologically different.
2. Even with all of the quantitative information extracted from a variety of evolving network pore structures, it has not been possible to determine unambiguously whether the fundamental mode of evolution is network coarsening, or network disconnection.

**EFFECT OF SINTERING ATMOSPHERE ON THE EVOLUTION OF
PORE NETWORKS DURING SINTERING OF COPPER POWDER**

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Sintering, as it has come to be known, is a geometric change in which a mass of separate particles becomes a coherent body. Like all other metallurgical processes which depend upon surface tension for their driving force, it is a topological process, based upon a system of changes in the surface contour and connectivity. As a matter of sintering practice, it is well known that the process is sensitive to the composition of the gaseous atmosphere of the sintering furnace, but the reason for this has not been identified.

The present study embodies the correlated pursuit of two related factors, namely, (1) the measurement of surface tension of copper in a broad spectrum of sintering atmospheres, and (2) an examination of the effect of gas atmosphere upon the microstructural evolution of the pore network during sintering. These have been accomplished by measuring the force of sintering and relating it to the surface tension through the measured curvature of the solid-void interface. The measurements indicate that argon, helium, nitrogen, chloride vapor and various mixtures of these gases produce relatively little effect upon the surface tension, except perhaps for carbon monoxide which lowered the surface tension significantly. All of these gases suppress the sintering force to some extent. The retarding effects are approximately proportional to the concentration in the gas mixtures. The results also show that gases have strong influence upon the evolution of the pore volume, surface area and total surface curvature of the connective pore network. In all cases, the effects are to

(diminish the microstructural change in comparison with that produced in hydrogen.

The role of the gases is seen, thus, to be in determining the specific rate of change of each of the geometric parameters. It is proposed that the atmospheres act by altering the competition between densification and surface rounding mechanisms during the first stage of sintering to establish different frameworks at the onset of the second stage of sintering.

THE DISTRIBUTION OF GRAIN SIZE AND FACES PER GRAIN DURING GRAIN GROWTH

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ABSTRACT

Although the topological model of grain growth is generally accepted as a necessary sequence of events for growth to occur, the model has never been extended to explain some of the interesting topological aspects of grain growth which have been observed experimentally. The present work reviews some of these observations of relationships between the distributions of grain size and of topological features and presents models describing this relationship and explaining the constancy of the distribution of faces per grain during grain growth.

Prior experimental observations have indicated that grain size distributions are generally well described by the lognormal distribution, as are the distributions of faces per grain and edges per grain face. In addition, the relative widths of these topological distributions, described by their geometric standard deviation, $\ln\sigma$, are observed to be proportional to the value of $\ln\bar{V}$ of the size distribution. During grain growth, the width of the size distribution remains essentially constant regardless of the initial value. This value of $\ln\bar{V}$ has been shown to be controllable, decreasing in value with increased percentage of cold work prior to recrystallization or increased solidification rate. The rate of grain growth, compared at constant mean grain size, has been shown to decrease with increasing

amounts of prior cold work, apparently due to the above effect of cold work on width of the grain size distribution and the resulting effects on the distributions of faces per grain and edges per face. Wider distributions of these topological features result in increased frequencies of 3-edged faces and 3 and 4-faced grains, which are the key features for grain growth, according to the topological model.

A new model has been developed to explain the previously mentioned relationship between the distributions of grain size and faces per grain. The model is based upon the numbers of grains of size j which can spatially surround other grains of size i , denoted $K(i,j)$ and illustrated schematically in Figure 1. Specifically $K(i,j)$ is the area of the spherical shell of diameter $(d_i + d_j)$ divided by the cross sectional area through an i^{th} sized grain. The number of faces on grains of the i^{th} class due to contact with j^{th} class grains among a distribution of other sizes, $F(i,j)$, is taken to be proportional to $V_V(j)$, the volume fraction of the j^{th} class:

$$F(i,j) = K(i,j) \cdot V_V(j) \quad [1]$$

Summing Eq. [1] over all m size classes yields $\bar{F}(i)$, the average number of faces on i^{th} class grains:

$$\bar{F}(i) = \sum_{j=1}^m [K(i,j) \cdot V_V(j)] \quad [2]$$

The average number of faces per grain, $\bar{F}$, is the average of $\bar{F}(i)$ over all classes:

$$\bar{F} = \sum_{i=1}^m [\bar{F}(i) \cdot N(i)] \quad [3]$$

where $N(i)$ is the number frequency of grains in the i^{th} class.

Figure 2 compares the distributions of faces per grain computed by the model for Hull's β -brass grains of known size distribution and the

experimentally observed distribution of faces. The model also yields a relationship between $F(d_i)$ and d_i related to the size distribution:

$$F(d_i) = A_1(d) \cdot d_i^2 + A_2(d) \cdot d_i + A_3 \quad [4]$$

where the $A(d)$ terms are functions of the width of the grain size distribution. Figure 3 illustrates this relationship computed for Hull's grains compared to his observed numbers of faces. Figure 4 illustrates the model prediction of increasing value of F with decreased distribution width, either by truncation or reduction in $\ln \sigma$. Figure 5 illustrates the relationship between $\ln \sigma(F)$ and $\ln \sigma(D)$ resulting from the model compared to experimental data from separated grains.

A second model describes the effects of grain growth, in terms of the loss of 3-edged faces, on the overall distribution of faces per grain. Two possible mechanisms for loss of 3-edged faces from the system, described by Rhines and Craig, are (I) direct loss of a 3 or 4-faced grains by shrinking to zero size and (II) loss of a 3-edged face by two adjoining grains pulling apart and losing contact. Figure 6 illustrates the numbers and percentages of 3-edged faces on grains with different total numbers of faces, $F(i)$, on separated aluminum grains. The number of 3-edged faces decreases from values of 3 and 4 to a minimum of 1.5 at $F = 8$ and then increases with increasing F value. The percentage of 3-edged faces decreases from 100 percent at $F = 3$ to approximately 12 percent at $F > 15$. The number per unit volume of 3-edged faces on separate grains of the i^{th} face class, F_V^{e3} is given by:

$$F_V^{e3}(i) = F(i) \cdot N_V(i) \cdot Z(i) \quad [5]$$

where $Z(i)$ is the fraction of 3-edged faces on grains in the i^{th} face class (Fig. 6) and $N_V(i)$ is the number of these grains per unit volume.

The total number of (separated) faces lost from the system, ΔF_V , during a small grain growth interval is:

$$\Delta F_V = 2[\Delta F_V(I) + \Delta F_V(II)] \quad [6]$$

where (I) and (II) indicate those faces lost by the type I and II events described above. All faces lost by either event are three-edged. If ΔN_V grains are removed from the system by disappearance of 3-faced grains, then the number of (separated) 3-edged faces on these grains lost from the system is:

$$\Delta F_V(I) = 3\Delta N_V \quad [7]$$

The loss of these grains also removes $\Delta F_V(I)$ faces from adjoining grains. These type I events plus the type II events which will also occur during grain growth cause a steady transfer of grains to lower face classes in the distribution. The sum of these separate faces which will be lost, ΔF_V^Q is then:

$$\Delta F_V^Q = \Delta F_V(I) + 2\Delta F_V(II) \quad [8a]$$

$$= \Delta F_V(I) + [\bar{F} \cdot \Delta N_V - 2\Delta F_V(I)] \quad [8b]$$

$$= 3\Delta N_V + [\bar{F} \cdot \Delta N_V - 2(3\Delta N_V)] \quad [8c]$$

$$= (\bar{F} - 3) \cdot \Delta N_V \quad [8d]$$

The number of grains moving from the i^{th} to $(i-1)$ class in a small interval of growth is:

$$Q(i) = F_V^{e3}(i) \cdot (\Delta F_V^Q / F_V^{e3}) \quad [9a]$$

$$= F(i) \cdot N_V(i) \cdot Z(i) \cdot (\Delta F_V^Q / F_V^{e3}) \quad [9b]$$

where

$$F_V^{e3} = \sum_{i=1}^n F(i) e3 \quad [10]$$

Equation [9] is based on the assumption that all three-edged faces, on

grains with more than 3 faces, have an equal probability of loss, regardless of the complexity of the grains forming the face. The change in the number of grains in a particular face class, $\Delta N_V(i)$, is equal to the difference between the number of grains moving into the i^{th} from the $(i+1)$ class and the number moving from the i^{th} to $(i-1)$ class:

$$\Delta N_V(i) = Q(i+1) - Q(i) \quad [11a]$$

$$= (\Delta F_V^Q / F_V^e) \cdot [N_V(i+1) \cdot F(i+1) \cdot Z(i+1) - N_V(i) \cdot F(i) \cdot Z(i)] \quad [11b]$$

and

$$\Delta N_V = Q(3) \quad [12]$$

After m growth iterations, the total number of grains lost, ΔN_V^{tot} , is:

$$\Delta N_V^{\text{tot}} = \sum_{j=1}^m [Q(3)]_j \quad [13]$$

and

$$N_V = \sum_{i=3}^n N_V(i) \quad [14a]$$

$$= N_V^0 - \Delta N_V^{\text{tot}} \quad [14b]$$

where N_V^0 is the initial value of N_V before growth.

The new value of $\bar{F}$ is then:

$$[15]$$

The above model was tested by computing the net change in $N_V(i)$ for each face class and the resulting distribution of faces for many successive growth iterations. Different starting distributions of faces per grain were tested, including lognormal, uniform, single valued and bimodal. all distributions eventually attained a lognormal form. Figure 7 illustrates the distribution of faces per grain after different numbers of growth iterations for a lognormal input distribution from experimental data. The form of the distribution remains essentially constant, with a mode at approximately 7, although the distribution narrowed slightly during grain growth. The value of $\bar{F}$ decreased slightly with grain growth.

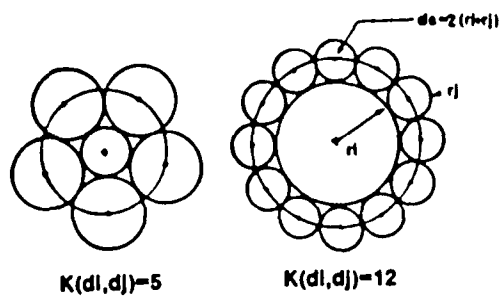


Figure 1. Two dimensional analogue of the three dimensional model of $K(d_i, d_j)$, the number of contacts on a central particle of diameter d_i from surrounding particles of diameter d_j .

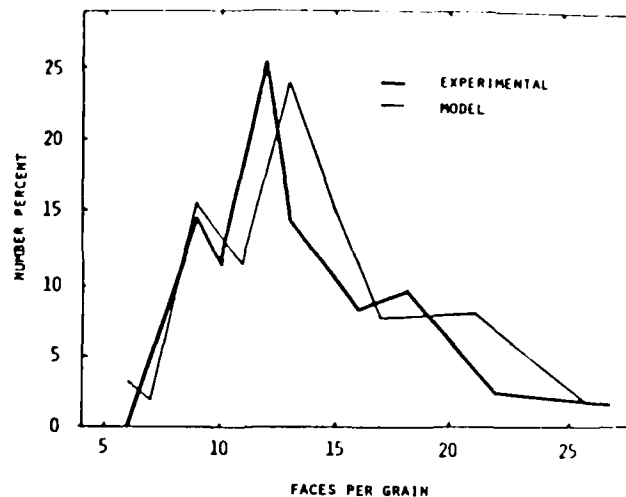


Figure 2. Comparison of experimental face per grain distribution for brass grains and the distribution predicted by the model.

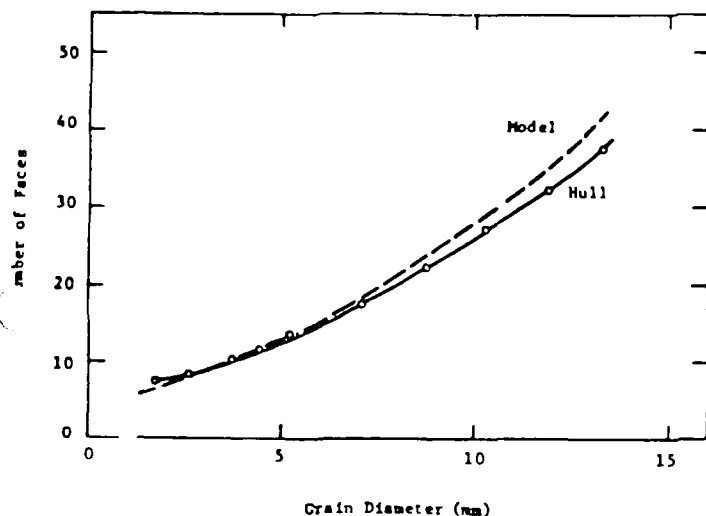


Figure 3. Relationship between the number of faces on grains and the grain diameter, predicted from the model and for experimental data.

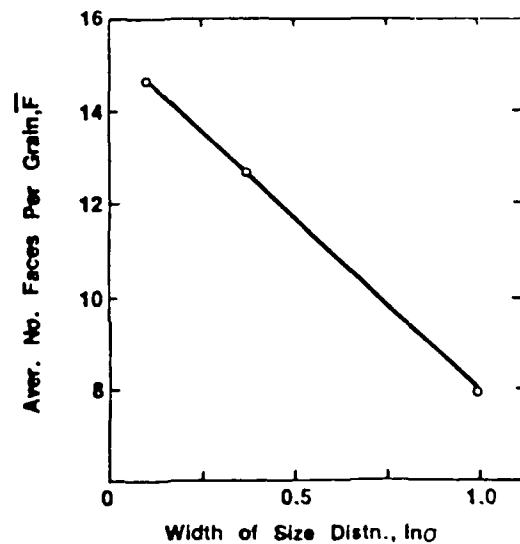


Figure 4. Effect of the width, $\ln \sigma$, of the grain size distribution on the average number of faces per grain, $\bar{F}$, at constant mean size and degree of truncation.

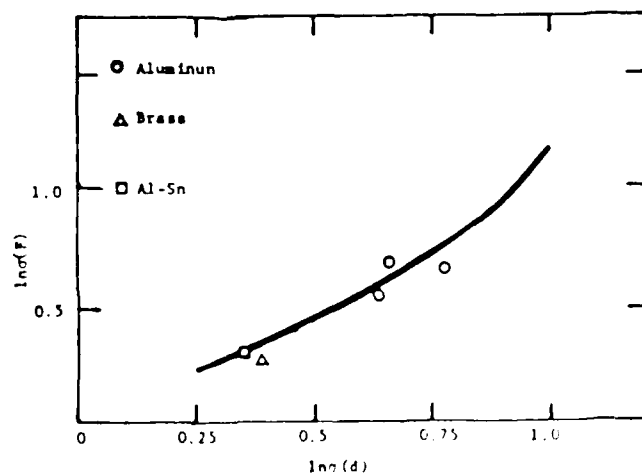


Figure 5. Relationship between $\ln \sigma(F)$ and $\ln \sigma(d)$, predicted from the model and from experimental data.

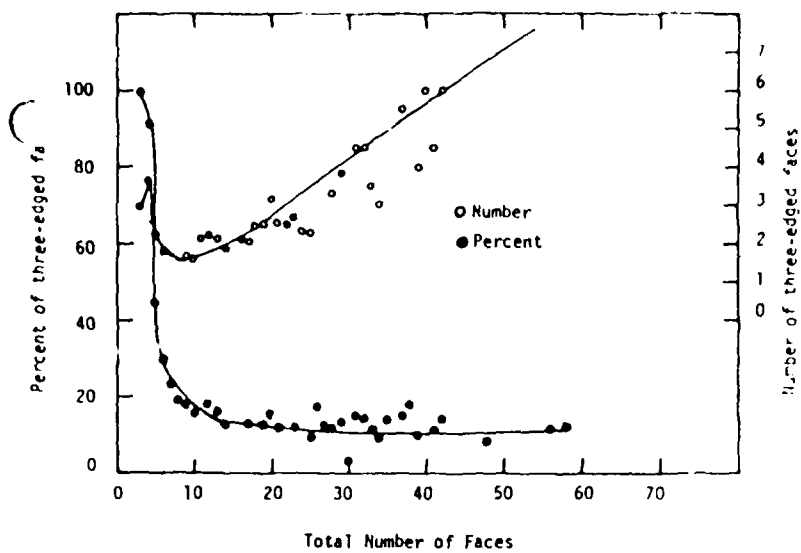


Figure 6. Number and percent of three-edged faces on grains of different numbers of total faces.

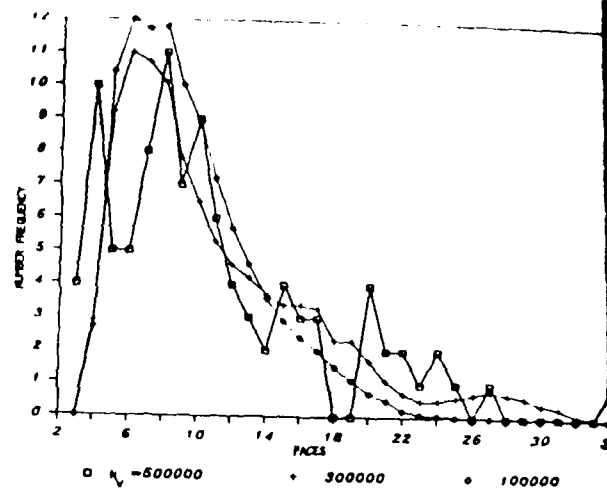


Figure 7. Predicted distributions of number of faces per grain at different degrees of grain growth (value of N_v) for a lognormal starting distribution.

Concern: International Conference on Microstructology Gainesville,
May '86/extended abstract

Microstructure-property correlations with respect to conductivity and
Youngs modulus of elasticity

Content of the presentation:

I. The problems background

Subdivision of structure and properties; definition of microstructure and field properties;

definition of aim: better insight into the materials behaviour (scientific) providing the basis for tailoring materials (technologically)

II. Theory of microstructure-property correlations

II.1 Conductivity

II.11 Bound concept

The bound concept leads to bound equations of different order depending on the available microstructural information. No geometrical assumptions are made. - For higher order bounds, however, no equations result from derivations unless geometrical suppositions are made. This is done, therefore in the

II.12 Model concept

based on spheroidal model mean values, the continuum principle and thermochemical equilibrium of the system (premises).

The resulting constitutive (model-) microstructure-field

property equations converge with the bound equations for respective microstructural parameters or factors.

II.2 Youngs Modulus of Elasticity

Again bound and constitution equations exist, again derived via a bound concept and a model concept.

And again convergency comes out for special limiting conditions, although the theoretical state-of-the-art for elastic constants and their relation to microstructure is still lower than that for field properties.

III. The determination of microstructural factors by quantitative microstructural analysis

Five microstructural parameters respectively factors dominate the properties.

Two parameters are implicit in the equations: the number of phases present in the system and the type of microstructure - matrix or interconnecting phases.

Three factors are explicitly appearing in the equations: the phase concentration factor, the shape factor, the orientation factor.

The phase concentration factor is a global parameter by nature.

The shape and orientation factors reduce to axial ratios by derivation.

If these axial ratios could be substituted by global lineal parameters the model would just play the role of a fictive aid to derive the equations. This question remains open yet.

IV. Comparison between calculated and measured values of field properties and Youngs modulus for real two-phase materials

IV.1 Conductivity

IV.2 Youngs Modulus

IV.3 Thermal shock resistance

Experimental conductivity and Youngs modulus data are compared with calculated values for all kinds of two-phase materials:

- metals and ceramics including glass
- cermets, metal-polymer- and polymer-ceramic-composites
- porous metals, ceramics and graphite

For the thermal shock resistance as a "technical property" composed by different terms of physical properties such as conductivity, Youngs modulus, rupture strength and the coefficient of thermal expansion a tentative consideration is made about microstructural effects.

Effect of Grain Volume Distribution On the Plastic Response of Aluminum Polycrystals

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Abstract

The plastic response of aluminum polycrystals, characterized by the yield stress, flow stress, work hardening, and the strain to fracture will be shown to be strongly dependent on the distribution of grain volumes.

The grain volume distributions were determined by embrittling aluminum polycrystals with liquid gallium penetration, followed by grain separation. In all cases, the grain volumes were found to be distributed log-normally. The grain volume distribution width, $\ln \sigma_g$, was used as a statistical descriptor of the microstructure.

It was determined that $\ln \sigma_g$ can be controlled by controlling the thermomechanical history of the sample. Also, $\ln \sigma_g$ remained approximately constant during steady-state grain growth. This information was used to produce a series of annealed samples with various values of $\ln \sigma_g$, but with the same grain boundary area per unit volume (S_v). The measured plastic response of these samples was then attributed to a variation in the $\ln \sigma_g$ values.

The yield and flow stresses were found to depend strongly on the grain volume distribution, and decreased monotonically with increasing $\ln \sigma_g$. The work hardening behavior (defined as the slope of the true stress - true strain curve) at constant stress also exhibited a strong dependence on $\ln \sigma_g$. The measured necking strains and the strains to fracture showed a fair amount of

(scatter; however, the trend indicated a tendency towards an early fracture at high distribution widths. The scatter in the data could be attributed partially to the statistical nature of necking.

A phenomenological description of this effect will be presented. The description is based on the fact that the S_v of a crystal is inversely proportional to its volume. It is proposed that the stress required to propagate shear through crystals (in a polycrystalline body) is directly proportional to their individual S_v 's. This argument leads to the conclusion that in a deforming polycrystal, there exists a distribution of apparent flow stresses which is inversely related to the distribution of grain volumes. Furthermore, the onset of plastic deformation produces an hierarchy of strains in the polycrystalline body, with the largest crystals deforming first, and also exhibiting the highest strain. This is supported by transmission Laue diffraction patterns of crystals separated from a deformed polycrystal.

(Thus, a global view of the deformation behavior in aluminum polycrystals is proposed, based on a statistical characterization of the microstructure.

SEMINAR on MICROSTRUCTOLOGY

Gainesville, Florida
7-9 May 1986

Title: Analysis of Fracture Roughness Parameters

Author: E. E. Underwood

Abstract:

Two simple, physically-meaningful roughness parameters for nonplanar surfaces are R_S , the surface roughness parameter, defined by

$$R_S = S/A'$$

where S is the actual area of the fracture surface and A' is its projected area, and R_L , the profile roughness parameter, defined by

$$R_L = L/L'$$

where L is the measured profile length and L' is its projected length.

R_L is experimentally accessible from vertical sections through the fracture surface, while R_S , the quantity desired (i.e., the true fracture surface area per unit projected area) is difficult to obtain.

Several investigators have proposed relationships between R_L and R_S that have the same form, but with different coefficients. An analysis of the various derivations reveals a misconception about the basic meaning of the stereological equations employed.

An alternate derivation is presented that avoids the pitfalls in other analyses, and which is based on the actual partially-oriented configuration of real fracture surfaces. Comparison with all available experimental data (Al-Cu, 4340 steel, Al_2O_3 ceramic) shows the best fit with the latter relationship.

The role of image analysis in stereology

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The impression which one may obtain by an examination of the technical literature in the field of stereology (which is rather confirmed by the manufacturer's brochures on commercial measurement systems) is that those measurements which can be automated are carried out on binary (discriminated) images. Grey images may be looked at by humans to mark, count or measure objects, and computer assistance may be used for record keeping or statistical analysis, but for automatic measurement purposes, it is thought necessary to find subjects which can be discriminated based on pixel brightness to delineate the objects of interest.

This impression is unfair. There are quite a number of measurements which can (sometimes must) be carried out on the grey-scale images, and an even greater diversity of "image processing" operations which can (sometimes must) be performed on the images to make them suitable for discrimination and measurement. This pre-processing also broadens the potential scope of application of stereological methods in several ways: permitting more "difficult" images to be automatically measured, and measuring parameters which characterize different aspects of objects' size, shape, morphology, etc.

The bulk of the work that will be described has been performed with a very small computer (Apple II with some enhancements to processor speed, memory, display and storage). With these systems attached to microscopes and video cameras, it is practical to perform image processing operations in the spatial domain (where each pixel's brightness is compared in various ways to its neighbors), and to combine operations on the binary images and grey images (e.g. to measure object brightnesses), but no work has yet been attempted on frequency domain processing (e.g. to remove blurring or sharpen images) or geometrical transforms (as used in spacecraft images to flatten surfaces viewed at non-normal incidence), and rarely has correlation averaging (combining multiple images of similar objects) been used. These have fortunately not been needed in our image analysis work using light microscope, TEM and SEM micrographs.

A major class of operations under the general heading of image processing modifies the brightness of each pixel based on its local neighborhood, in ways that improve the ability to automatically distinguish objects from their surroundings, or to separate them from other, touching objects. This field is generally called "segmentation" and is actively under development in the machine vision and robotics field as a precursor to identification of objects in images. The most commonly known methods involve applying local operators to reduce the brightness differences between pixels within a single object (smoothing), and to calculate the Laplacian (gradient) of an image to locate edges. Both methods introduce serious distortions or noise into real images, which frustrate subsequent measurements. The use of a median filter is far superior to the traditional smoothing operator, as it does not displace or reduce the brightness magnitude across edges. Sobel and Kirsch operators

which find either the maximum or rms gradient, define edges without introducing noise, and are particularly powerful for segmenting complex images in which different objects have overlapping grey scale values. Several examples will be shown, and efficient computational schemes described. More aggressive methods, such as the Hough transform, region growing, and edge tracking, have been used in a few cases. However, they require substantially more computing time and fail catastrophically for some images.

Averaging the brightness of pixels (in the original image) lying within a feature boundary (perhaps obtained by the methods just described) is commonly used to obtain a mean density value for features viewed in transmission (in light or electron microscopes). Less common are methods which examine the texture of surfaces viewed in the SEM. Plots of the difference in pixel brightness as a function of distance between pixels lying within an object provide two parameters (the slope and intercept of the curve) which are often able to distinguish object types in ways that appear to mimic human visual recognition of roughness and texture. Whether the parameters correlate with other "real" measures of surface roughness, such as fractal dimensions or wrinkle factors, remains to be studied. We have been determining the fractal dimension of feature outlines using a coarsening method, which is both fast and accurate and has proven itself able to provide feature recognition independent of size and orientation.

Another use of the brightness of pixels within individual features is for adaptive thresholding. In many images (perhaps due to nonuniform illumination, sample thickness or camera response) the background (the region outside the features of interest) does not have a uniform brightness level. In addition, the features themselves may vary. Consequently there may not be any global discriminator level that will properly define the features. This can be partly overcome by fitting global correction functions to the background to level the image. A more tedious but flexible scheme is to examine the brightness of pixels along the periphery of each object, as determined by a first-approximation discriminator level. These are then assigned to the feature or the surroundings based on comparison to the local neighborhood or feature mean brightness. This is similar to the way human vision operates, which can distinguish features in the presence of severe shading and variation in overall brightness. The result provides segmentation of the image features with fewer cases of touching or breakup of objects than global discrimination, and thus allows automatic measurement of images which would otherwise require human delineation. It appears to be superior to, although requiring more computation than methods which use the minimum in the brightness histogram, or the midpoint between the maxima, or the plot of perimeter vs. discriminator level. None of these methods can be applied blindly, however, as there are numerous images for which each fails.

Finally, when measurements on a discriminated ("binary") image of objects are carried out, the parameters which can be efficiently determined by the computer-based system are usually not those which are of direct interest to the user. The area, perimeter (limited in accuracy by the pixel dimensions), minimum and maximum projected (Feret) diameters, mean intercept length, location and orientation, convex ("taut string") perimeter, fractal dimension of the profile, net tangent count ("profile curvature"), number of internal holes ("connectivity"), and the mean brightness and texture mentioned above, can be determined for each object in the field of view. At somewhat greater cost in computational complexity, the number of ends and nodes of the skeleton can be obtained. From these

measured parameters, models must be used to estimate the dimensions and shape of the generating object. These models are different for sections through objects (e.g. metallographic specimens observed in the incident light microscope) and for projected images (e.g. particulates viewed in TEM or SEM); particularly for the latter case, these models introduce some bias. We have used Monte-Carlo simulation to evaluate ellipsoidal models for convex objects, and fiber models. Better estimators, and probably some "artificial intelligence" rules to select the most appropriate ones for a given class of object, are urgently needed. The key indicators of object "class" seem to be formfactor ($4 \pi \text{ area} / \text{perimeter}^2$), coverage (projected feature area / min-max projected diameter), and aspect ratio (max / min projected diameter). The desired "derived" parameters include volume and surface area, fiber length and diameter, and estimates of topological shape descriptors.

Another class of images that will be discussed briefly is direct three-dimensional images. These include stereo pair photos from the SEM, serial section images from the TEM, depth-controlled ("optical" sectioning) images from the scanning acoustic microscope, and sequences of element-specific images as a function of (mostly) depth from the Ion Microprobe. Work is just beginning as well on 3-D reconstruction of images obtained from the TEM at a series of specimen tilt angles (roughly analogous to CAT scans). Each of these topics has required some ad-hoc methods development. For instance, stereo pair photos do not usually contain identifiable merge points in any sort of regular grid. Faced with a random arrangement of points whose elevations are known from the parallax in the two images, we have devised computationally efficient ways to triangulate the plane, interpolate a contour elevation map, and proceed to integration of volumes. As another example, SIMS images from the Ion Microprobe can readily be viewed in simulated 3-D, and elemental concentrations and ratios along any profile or section plane can be studied, but corrections for differential sputtering rates are made only by manual realignment of portions of the sections. Nevertheless, these methods appear to provide useful ways to characterize and sometimes measure 3-D structures.

I believe that there is an important role for these kinds of image processing operations as an adjunct to stereological measurements. The amount of computer power required is modest, and the times required tolerably short (from a few seconds to about 15 seconds) for images with 256 pixel widths. The equipment required is sufficiently inexpensive to permit attaching dedicated systems to various microscopes in the laboratory, and these may also be used for the various measurement and statistical functions.

INTERNATIONAL CONFERENCE ON MICROSTRUCTOLOGY
Department of Materials Science and Engineering, University of Florida
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INEXPENSIVE SYSTEM FOR MEASUREMENT OF STEREOLOGICAL PARAMETERS

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In materials science it is extremely important to obtain correlations between microstructure and physical properties of materials. Several kinds of parameters can be used to describe quantitatively the microstructure. Among the stereological parameters, the volumic fraction, the specific surface area, the mean curvature and the length of lineal features are accessible by simple counting. It can be done automatically with most of automatic image analyzers available on the market. Unfortunately, these apparatus require an automatic thresholding of the images and this is not necessarily obvious or even possible. Moreover, these equipments are very expensive.

So, it seemed us useful to develop a system semi-automatic (in order to avoid the problems associated with the threshold), easily available and inexpensive. The overall system requires a camera, a microcomputer with two disk-drives and a digitization table or a mouse (it is originally implemented with an Apple IIe). The basic idea is to superimpose on the TV monitor the image from the camera and (for example) a grid of points synthesized in the microcomputer's memory. The two electronic signals coming from the camera and from the microcomputer are mixed in a "connector" and sent to the TV monitor. The cursor of the digitization table or the mouse is used to select the points (for example, count the points inside one phase). The results (basic stereological parameters) and their statistical treatment are displayed at the end of analysis and can be sent to a printer.

The description of the software and the electronic scheme of the "connector" will be given here.

ESTIMATION OF GROWTH RATES FOR PARTICLES AS PARTS OF A SYSTEM

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Introduction

This paper shows the results of the application of the growth path approach of graphical construction to the estimation of growth rates for particles in several Al-Si alloys during isothermal treatment. The analysis presented here shows the process of growth of silicon particles in an aluminum matrix from a different point of view from that already shown by the authors for the same material (1), and its main purpose is to enhance the differences when a same process is perceived as a whole system and as a set of classes which can individually exhibit different behaviour. It emphasizes the well established view that some phenomena should be treated differently when viewed as global processes rather than a simple aggregation of parts.

Experimental procedure

The alloys and temperatures of treatment are shown in table I. The procedure for preparation of the material and samples has already been described (1) The measurement of particle size distributions has been carried out after dissolution of the matrix in a water-hydrochloric acid mixture, and the extracted particles have been run through a Coulter counter to derive the actual particle volume distributions. Times of treatment ranged between 20 and 2500 h.

Table I. Silicon content of alloys and thermal treatments

Si, wt%	4	4	7	7	7	7	12	12
Na-modified	*		*	*	*		*	
Temperature °C	540	540	500	540	566	540	540	540

Results and discussion

All values shown have been produced using the particle size distributions obtained by the procedure described above, what we call "size" in this occasion is actually an arithmetical mean volume as deduced from the mentioned data

A typical distribution of particles is normally represented as a plot of cumulative percentage of the total number per unit volume, N_v , vs size class for normal distributions, and vs log size class for lognormal distributions. For the purpose of the present analysis, however, they are plotted as log number per unit volume vs log size class (2), as shown in Fig 1 for an ideal case. For a set of such plots drawn from data corresponding to different times it is possible to find out for a constant number of particles (N_v , terminology according to (2)) different growth paths (Fig 2), which together constitute the growth path envelope. The significance of an individual growth path would be that of the evolution of the size (volume) of a given particle, or rather

given size class, with time, for constant temperature. The procedure has been described by DeHoff(2) and has been applied in a number of occasions (3), but seldom on volumes, the main advantage of this latter approach would be to avoid assumptions about the shape of particles. A set of N_v -constant values vs time curves allows a complete set of growth paths to be constructed. From this construction it is straightforward to find out a new set of values, namely volume vs growth rate tables. An interesting outcome of these figures is that if growth rates are plotted vs volumes, the data for different times show different linear relations (Fig 3). To estimate whether there is a reasonable approximation to linear relations of this type, it seems adequate to find out the correlation coefficients for the set of v vs dv/dt values. Fig 4 shows the distribution of such coefficients. 40% are between .99 and 1, 62% are higher than 0.95 and about 10% are lower than .80. There is then a reasonable indication that growth rates are proportional to particle volumes for a given treatment time, a vertical line which indicates a given growth rate, then, would show larger volumes to correspond to longer times. On the other hand, the spread in growth rates decreases with time.

Critical volumes

The notion of critical size, or, more adequately, critical volume, is that of a size which represents particles which would not be growing or shrinking. These "critical" volumes can also be derived from the same set of growth paths for values $dv/dt = 0$.

If the system is considered as a whole, it becomes clear that there may not be such thing as a "critical" particle, the fact that a particle grows or shrinks will not only be determined by its size at a given moment, but also by the size of its neighbors. Critical volumes obtained in that way should then be viewed as "average" critical volumes rather than physically significant quantities. With this limitation in mind it is also possible to construct a table of critical volumes. Preliminary values have been obtained graphically, and there is an indication that no formal relation can be established between composition and critical volumes; it seems to depend more on the time of treatment, obviously this is difficult to explain, but might indicate that, as is the case with the system considered as a whole, that parameter is determined by the global state of the system.

These are only some incomplete observations of what may be happening when particles are considered individually instead of as a system (as has been done in (1)), this would show that the system as an interacting ensemble is behaving in a way that apparently cannot be modelled by the addition of the behaviour of individual particles.

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- 3 J.L. Chermant and M. Coster. Proceed. IV International congress for stereology. NBS sp. publ. 431. Washington, 1976. 287-290.

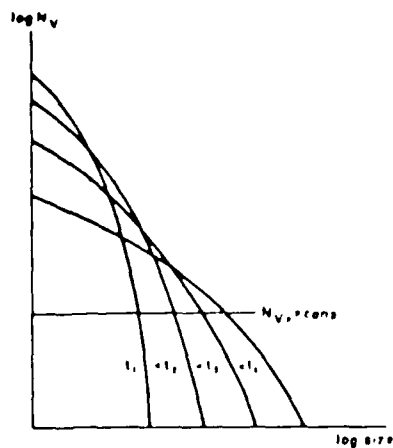


Fig 1. Derivation of N_V values for an ideal set of particle distributions.

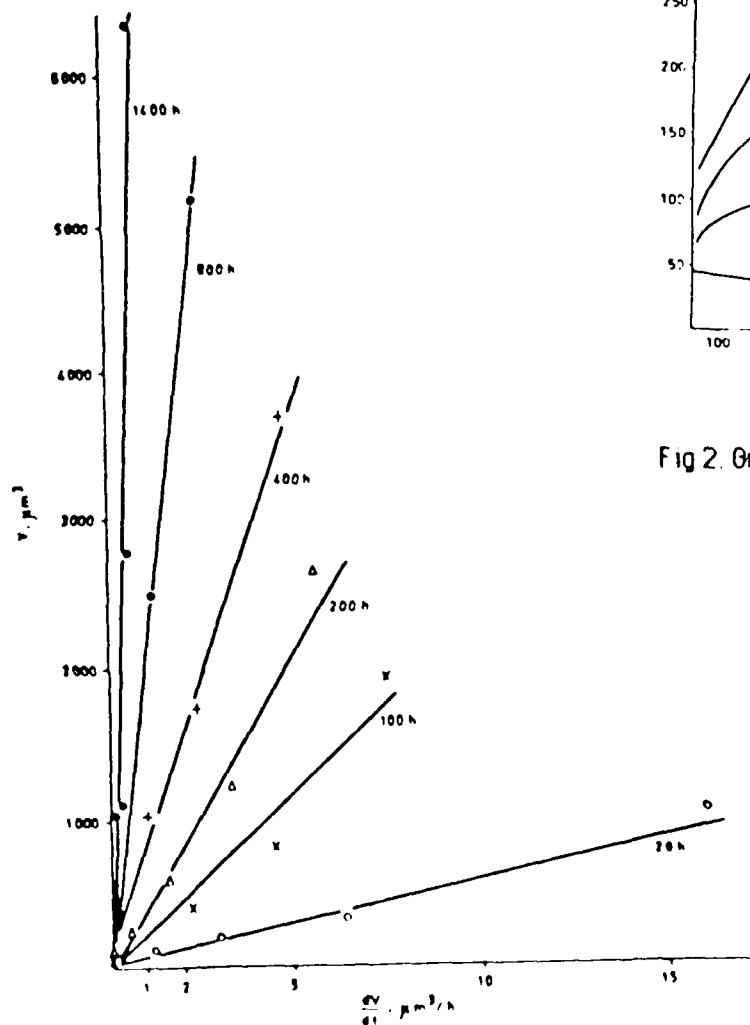


Fig 3. Volume vs growth rates for particles in Fig 2

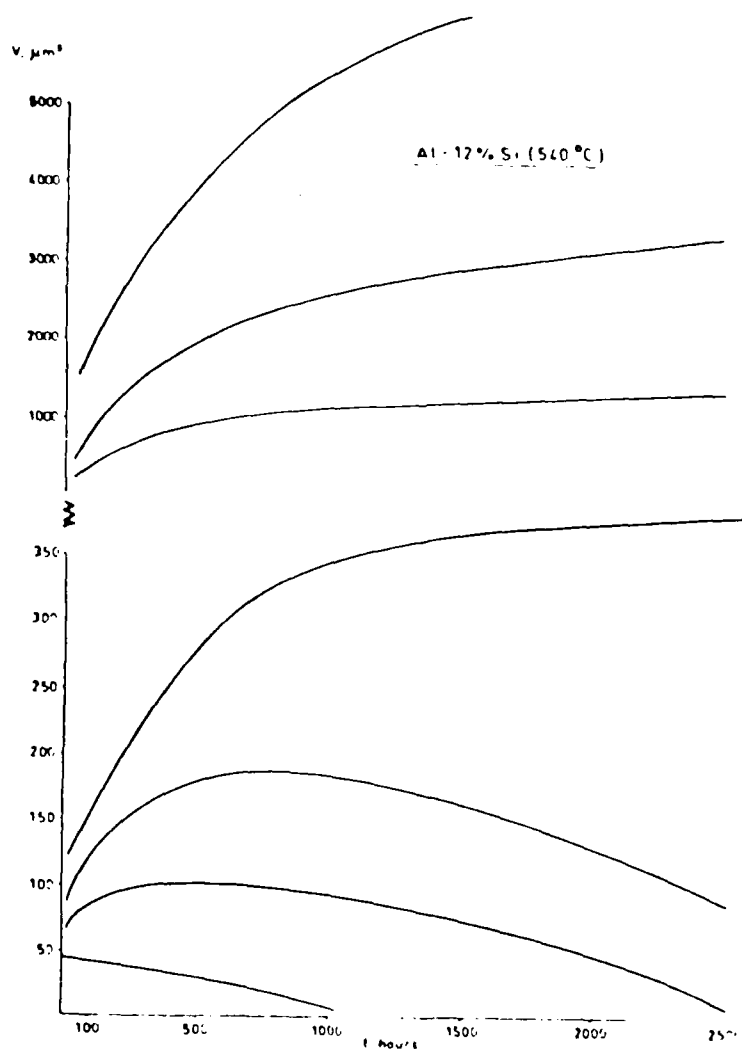


Fig 2. Growth paths for particles in Al-12%Si treated at 540°C

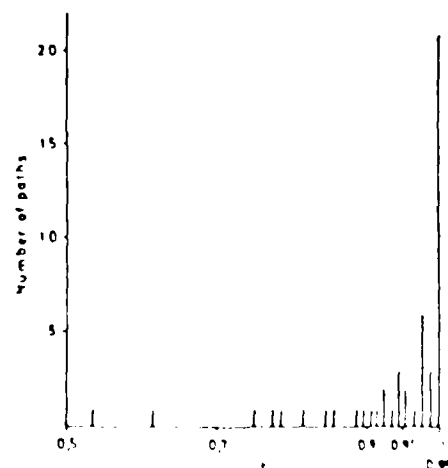


Fig 4. Distribution of correlation coefficients for all v vs dv/dt values.

TOWARD A GENERAL THEORY OF MICROSTRUCTURAL EVOLUTION

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Quantitative stereology provides the basis for the geometric characterization of the microstructural state of a material system. For any process, the path of microstructural change, i.e., the sequence of microstructural states traversed, provides rudimentary insight into some aspects of the evolutionary process. There exists a set of kinematic equations, termed interface displacement equations, which connect rates of change of the global microstructural state properties in a process to the distribution of local interface velocities:

$$\frac{dV}{dt} = \iint_S v dS$$

$$\frac{ds}{dt} = 2 \iint_S v H dS = 2 \iint_M v dM \quad \left[H = \frac{1}{2} \left(\frac{1}{r_1} + \frac{1}{r_2} \right) \right]$$

$$\frac{dM}{dt} = \iint_S v K dS = \iint_\Omega v d\Omega \quad \left[K = \frac{1}{r_1} \cdot \frac{1}{r_2} \right]$$

In these equations, V is the volume of the phase of interest, S is the area of its bounding surface, M is its integral mean curvature, and Ω is its spherical image. H is the local mean surface curvature of a surface element, K is the local Gaussian curvature, and v is the local (normal) interface velocity.

The connection between the stereologically determined global geometric properties and the kinetics governing the microstructural process (i.e., the physics of the situation), is made through the evaluation of v , the local interface velocity, in terms of the material flows that produce local interface displacement. Where such an evaluation can be made without simplifying

(geometric assumptions, the resulting theoretical description of microstructural evolution may be termed geometrically general.

This approach has been applied theoretically to some classes of microstructural processes, including: control of coarsening by interface reaction kinetics; control of evolution by surface diffusion; control by volume diffusion in the phases adjacent to the advancing interface; and, with some assumptions, sintering. Predictions of the resulting theories are not always couched in terms that are stereologically accessible. Nonetheless, the results are free of geometric assumptions and, at the very least, display the kinds of geometric properties that must be sought in order to make definitive tests of kinetic assumptions.

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APPENDIX B

Questionnaire Circulated to Participants

INTERNATIONAL CONFERENCE ON MICROSTRUCTOLOGY

University of Florida
Gainesville, Florida

May 7-9, 1986

In order to jog your memory, a program accompanies this sheet, with each of the presentations assigned a number.

1. Please list by number the presentations that you found:

- a. Most interesting _____
- b. Consistent with the objectives _____
- c. Inconsistent with the objectives _____
- d. Otherwise noteworthy _____

2. Please supply your reactions to the following statements (be candid):

- a. At the present state of the art, materials science is largely a qualitative science.

- b. The use of realistic, unambiguous geometric concepts in the study of microstructures in processing and properties is vital to the ultimate development of a quantitative materials science.

- c. It is essential that we initiate and foster the development of a shift toward the use of realistic and unambiguous geometric concepts in those aspects of materials science research that center around the role of microstructure.

Signature (optional)

INTERNATIONAL CONFERENCE ON MICROSTRUCTOLOGY

Program

1. F. N. Rhines and R. T. DeHoff - "Basis of Microstructology"
2. H. E. Exner - "Shape: A Key Problem in Quantifying Microstructure"
3. H. Gundersen - "Quantitation of Microstructures without Geometric Assumptions"
4. O. Richmond - "Space Tessellations for NonRandom Points and Particles"
5. B. Ralph - "Factors Controlling the Evolution of Grain Size During Grain Growth"
6. H. Conrad - "Effect of an Electric Current During Recrystallization on the Size and Shape Distribution of the Resulting Grains"
7. C. S. Smith - "Toward a Philosophy of Structural Change"
8. R. W. Cahn - "Antiphase Domain Boundaries, Grain Boundaries and the Ductility of Alloys"
9. M. E. Glicksman - "Evolution of Microstructural Length Scales"
10. R. T. DeHoff - "Evolution of Porous Network Structures in Powder Processing"
11. S. S. Chang - "Effect of Sintering Atmosphere on the Evolution of Pore Networks During Sintering of Copper Powder"
12. B. R. Patterson - "The Distribution of Grain Size and Faces per Grain During Grain Growth"
13. G. Ondracek - "Microstructure-Property Correlations with Respect to Conductivity and Young's Modulus of Elasticity"
14. A. Gokhale and F. N. Rhines - "Effect of Grain Volume Distribution on the Plastic Response of Aluminum Polycrystals"
15. E. E. Underwood - "Analysis of Fracture Roughness Parameters"
16. J. H. Steele - "Microstructure-Fracture Correlation - A Pandora's Box"
17. J. C. Russ - "The Role of Image Analysis in Stereology"
18. J. P. Jernot - "Inexpensive System for Measurement of Stereological Parameters"
19. F. N. Rhines and M. Aballe - "Estimation of Growth Rates for Particles as Parts of a System"
20. R. T. DeHoff - "Toward a General Theory of Microstructural Evolution"

APPENDIX C

Comments

The following are excerpts from responses to the questions posed to the participants as shown in Appendix B.

2a. At the present state of the art, materials science is largely a qualitative science.

C. S. Smith: To a fair extent, but doesn't it have to be? The very nature of MSE is that it is at the interface between quantitative atomic behavior at small scales of structure, merging into the full complexity of polyphase aggregates fitted by human trial to external requirements. This is not exact geometry but is topology with inevitably many alternate routes to closure and interpenetration of connection, flow and shear and thermal (and social!) fluctuations.

M. E. Glicksman: I agree. The areas where serious attempts are underway to bridge the gap to rigorous paradigms are limited. Where such activity is underway, with materials scientists working with mathematicians/physicists, enormous strides are being taken.

R. W. Cahn: If you had said that materials science incorporates an inescapable residue of empirical (i.e., non-analytical) activity, I should have agreed. But taken as a whole, materials science is no longer qualitative and stereological analysis has directly contributed to this development.

M. Aballe: This is absolutely true for the part of Materials Science mostly related to microstructure and its evaluation. Other areas (diffusion, point defects, equilibrium diagrams) are more quantitative. Mechanical properties are somehow in the middle.

Anonymous: Subdividing engineering materials science into four major parts - structure, properties, technology and quality control - there exist several quantitative correlations (e.g., calculating phase diagrams, surface and interface energies, magnetic behavior from atomistic principles, etc.). But the key position for "constructing tailor-made materials," the microstructure-property correlation, is not yet in the desired quantitative state.

B. Ralph: Too sweeping but tends to be true of some areas, particularly much of the microscopy field.

B. R. Patterson: More for some areas, such as microstructural studies, than others. The microstructurally related areas are still very much qualitative due to the general lack of understanding among researchers of methods for quantifying microstructural properties.

J. C. Russ: I would modify the statement to read: "As practiced by most academic and nearly all industrial scientists, Materials Science is largely a qualitative science." True. The state of the art permits a fair number of quantitative lessons to be drawn and the hope for the future is towards more such capability. The aim of most of the attendees at the workshop was to develop such new methods and apply them to their specific areas of research. How these techniques will diffuse to the community at large is a more difficult subject not yet addressed. If they can be embodied in measurement devices, they are more likely to be used than if every metallurgist has to understand mathematical topology!

2a. (continued)

H. Conrad: I would say semi-quantitative rather than qualitative.

H. E. Exner: Holds only for those aspects of materials science which deal with the complex interactions of processes and parameters in materials. There is a large number of unitary models which treat isolated problems qualitatively (but hardly anything both quantitatively worked through and consistent with observations).

J. H. Steele: Not true - quantitative in many theories and qualitative in others. This overstates the case, implying almost every theory in materials science is qualitative?

- 2b. The use of realistic, unambiguous geometric concepts in the study of microstructures in processing and properties is vital to the ultimate development of a quantitative materials science.

C. S. Smith: Only if you want a straight-jacket that will stifle new development, but perhaps that's what you mean by "ultimate," which is changeless. What is needed is topology, not plane-faced Euclidean geometry. The only non-ambiguous feature of a structure is inclusion or exclusion of a junction/separation.

M. E. Glicksman: I strongly believe that materials science will always tend to bifurcate: qualitative microstructure analysis assisting the "descriptive" approaches toward materials science; quantitative unambiguous methods required for true scientific advances in our field. The two shall co-exist!

H. E. Exner: Yes, but it is also vital to intermediate stages of developments of materials science. Sorting out useless unitary models, unifying ways of descriptions and measurements for microstructures in order to make results comparable (e.g., using "surface density" instead of undefined "size").

B. Ralph: Absolutely. However, many of these geometric concepts are relatively difficult to apply. We need them translated so they may be applied more routinely. This involves both a modification in the presentation of the concepts and a considerable effort on the education front.

Anonymous: This statement is correct but needs to define the term "realistic." Realistic is what the correlation between properties and microstructure reflects in a proper way but not necessarily what describes reality in a geometrically most real way!

M. Aballe: I agree completely.

H. Conrad: Most definitely.

J. C. Russ: I strongly agree with the caution that not all materials science needs to be quantitative. Qualitative differences between materials, microstructures and methods are also important. As I understand the difference, quantitative methods will allow us to describe certain aspects or parameters with numbers and by implication with precision. Finding qualitative differences is the process of recognizing which parameters or aspects are important and perhaps should be measured. Sometimes this is either very easy or suggests itself as part of the measurement process. Often it requires an extreme amount of discernment and judgment on the part of the scientist. The easy parameters are mostly in hand now and we need new qualitative ideas to progress. Perhaps you intend this to be included in microstructology but I think that concern with purely global parameters which do not require shape assumptions may overlook part of this qualitative aspect of things.

B. R. Latterson: We have all seen far more examples of progress held back by use of unmeaningful, non-quantifiable measurements than of progress made by use of realistic parameters. It almost seems like anytime a breakthrough occurs, it is due to someone finally quantifying the correct parameters that had not been systematically measured before.

2b. (continued)

J. H. Steele: Quantitative materials science? If I can write a partial differential equation and solve it given realistic boundary conditions and find answers which fit experimental data, am I not quantitative (?)

R. W. Cahn: Not all of materials science relates to microstructure, though a large proportion of it does. For that large proportion, this statement is entirely correct.

2c. It is essential that we initiate and foster the development of a shift toward the use of realistic and unambiguous geometric concepts in those aspects of materials science research that center around the role of microstructure.

C. S. Smith: (See above - you can't do it. The whole virtue and value of microstructure is that it is scale dependent, with the boundaries between scales always ambiguous.) I enormously enjoyed the conference and was greatly stimulated by both papers and discussion. It did reinforce my inclination to believe that microstructure incorporates aspects of density within regions definable only by granular boundaries at some scale, very much like color, where little steps in density (frequency in time or granularity, and nothing) can affect response to external probes. Structural inertia merges into mass (gravitational) inertia. Density is qualitative: it's not affected by shape or size of boundary until the granularity of the boundary becomes significant.

M. E. Glicksman: Consistent with my view in part 2b, it is ABSOLUTELY! essential that rigorous theories and measures of microstructure be forthcoming. I'd go so far as to say that without the rigorous paradigms we don't know what microstructures really are, nor do we know how to manipulate or optimize them. Traditional metallurgy just does a fine job approximating the ideal.

B. Ralph: Yes. I wouldn't modify this statement at all. We need to build this science into our instruction program and that suggests we need new texts on microstructure which include quantification as well as phase transformations, properties, etc.

R. W. Cahn: The foundation has been done, much of it at the University of Florida. Yes, fostering it is essential and the best way by far to do that is to demonstrate these concepts in action. Continue to operate on the principle "don't do as I say, do as I do"! Our little meeting will have contributed to that and built on the lead provided by the admirable Rhines booklet.

H. E. Exner: Yes, absolutely. A first step would be to sort out ambiguous, superfluous and unnecessary complicated microstructural parameters and to define the useful ones (education of a larger number of people to use them). A small group could be formed uniting present diversification of "schools" (Florida, Caen...?). "Modelling" should follow the lines demonstrated by DeHoff.

M. Aballe: I agree completely.

H. Conrad: Most definitely.

B. R. Patterson: This is, of course, true. It is surprising, however, that even some of the attendees at the first Microstructology meeting did not employ rigorous descriptors in their work. It is certainly up to this group and others to take a more aggressive Rhinesean posture with regard to the use and misuse of realistic, quantifiable parameters in materials research.

J. C. Russ: It is necessary but not sufficient. In other words, I agree that the development of unambiguous geometrically unbiased measures of structure is a requirement for performing materials science research on the relationships between structure and properties on the one hand, and with processing variables on the other. But there is also a role for other techniques, some of which do

2c. (continued)

J. C. Russ (continued): make biasing geometrical assumptions. This is particularly true in the case of near-surface phenomena such as electronic materials. I feel more comfortable with the tenets of "microstructology" in a bulk environment.

J. H. Steele: Yes, but the past is not completely unrealistic? and not completely unambiguous?

Anonymous: There exists a number of central subjects in materials science in which microstructure plays a key role. Since they may concern materials in equilibrium (kinetics), for example, or problems in which materials may be treated as a continuation or where the weakest link is decisive, the geometric concepts have to take into account the aim, right from the beginning, and to be as simple as possible with respect to an engineering approach.

END

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