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6. AUTHOR(S)
David P. Pope and Vaclav Vitek

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Pennsylvania
Room 200 LRSM
3231 Walnut Street
Philadelphia, PA 19104-6272

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This is the final report for this program. Progress was made both on the experimental and theoretical aspects of the program. The experimental results demonstrate that single- and polycrystalline Al_3Ti in the $L1_2$ form (by adding Fe or Cr) is intrinsically brittle; although second phase particles can make it even more brittle. The theoretical portion of the program has produced a new theory of the brittle-to-ductile transition temperature involving dislocation-screening assisted homogeneous dislocation nucleation at the transition. The model provides realistic values of the transition temperature and reduces to the well-known Rice-Thomson model at zero temperature and to the equally well-known Kosterlitz-Thouless model at zero stress.

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Mechanism of Quasi-Brittle Failure in Metals and Intermetallic Compounds

D. P. Pope and V. Vitek
University of Pennsylvania
Department of Materials Science & Engineering
Philadelphia, PA 19104-6272

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1. Introduction

1.1 Statement of the Problem: Quasi-Brittle Fracture.

Failure of a structural component by unstable crack propagation is always a catastrophic event and, therefore, the development of materials which are not prone to this kind of breakdown has historically been a major occupation of materials scientists. Notwithstanding, a number of engineering structural materials are well known to be susceptible to such failure although they may possess at the same time relatively high ductility. The best known examples are bcc metals, in general, and iron-based (bcc) alloys, in particular. In such materials the mode of crack propagation is either transgranular, by cleavage, or intergranular, usually along prior austenitic grain boundaries embrittled by the segregation of impurities. Yet, in either case the failure is not totally brittle because even though the overall ductility observed in the fractured sample may be low, there tends to be large amount of inelastic deformation in the region localized around the crack. In such cases, although the fracture surface appears visually as corresponding to a totally brittle cracking, the work to fracture, extracted from the Griffith equation, can be ten or even hundred times higher than the true surface energy. Such fracture processes have been called quasi-brittle by Hack *et al* (1989) to distinguish them from truly brittle processes as occurring, for example, in silicate glasses. As discussed below, brittle intermetallic compounds belong to this category of materials and thus to attain a fundamental understanding of their mechanical behavior we have to tackle the generic problem of quasi-brittle fracture.

Developing a physical understanding of the mechanisms of quasi-brittle failure has been very slow because it is a combined problem of explaining why, on the one hand, the local stresses at a crack tip are sufficiently high to cause bond breaking but, on the other hand, there is not enough dislocation motion to bring about crack blunting thereby stopping the crack, even though the material is plastically deformable. A major step in understanding these processes was made by the observation that the process of brittle cracking in iron is *intrinsically a dynamic process* that involves microstructural features in a critical way (McMahon and Cohen 1965). It was realized that the extension of a cleavage crack from a notch or pre-existing crack is not a continuous process. Rather, upon loading, microcracks are nucleated at brittle inclusions ahead of the notch and propagate into the ferrite matrix, linking up to the main crack and causing overall failure. Most important is the finding that *pre-existing cracks* on inclusions *do not lead to failure,* since such cracks simply blunt by normal dislocation plasticity. Only those microcracks formed during the loading which are, therefore, dynamically injected into the matrix from the inclusions, actually contribute to brittle failure. This observation clearly demonstrates the essentially *dynamic nature* of cleavage cracking in a quasi-brittle material.

1.2 Models for quasi-brittle fracture

The most widely used model for analyzing cleavage crack initiation is that of Rice and Thomson (1974), in which the process of crack extension and dislocation emission from the crack tip are regarded as competing, mutually exclusive processes. Either local plasticity (dislocation emission) evolves at the crack tip and the crack remains stationary or there is no plastic deformation at the crack tip and the crack starts to propagate in a brittle manner. The model has been subsequently modified and refined in a number of ways (Mason, 1979; Thomson, 1978; Weertman, 1978; Thomson 1986; Bartholomeuz and Wert, 1991), but the essential features remain the same, viz, crack extension and local plasticity are viewed as mutually exclusive events.

The essential feature of the model is the assumption that the energy barrier for dislocation emission from the crack tip is a measure of the tendency for brittle failure. If the energy barrier is low or non-existent, dislocations are produced, thereby preventing crack propagation. In contrast, if the barrier is high, the crack does propagate. The barrier may be high, for example, if the free surface energy is high, or the shear modulus is very large or the Burgers vector of the dislocation emitted is especially long as, for example, in the case of undissociated superdislocations in compounds. However, in quasi brittle materials the work to fracture is always large compared to true surface energies (Knott 1977, 1987) which suggests that cracking and inelastic deformation are concomitant, rather than mutually exclusive processes.

A second point of view is dislocation mobility-controlled models of the BDT which have been proposed by several authors who considered the strain-rate dependence of T_c and its correlation with dislocation mobility as the dominant characteristic of the BDT (Brede and Haasen 1988; Hirsch *et al.* 1989; Nitzsche and Hsia 1994). Most of the mobility-based models involve numerical simulation of the dislocation dynamics in the vicinity of the crack tip. In contrast with the nucleation-controlled models, dislocation emission is assumed to be easy and a suitable criterion which enables the emission is imposed in the mobility-based models. For example, Hirsch *et al.* (1989) first assume that an avalanche of dislocations is emitted very close to T_c in order to reproduce the extremely sharp transition observed in Si (St. John 1975). A closer examination of the simulations reveals that the sudden transition is essentially caused by the introduction of the avalanche of dislocations and not by any mobility-related effects. Since the dislocation nucleation criterion is prescribed in an ad hoc manner it is not clear whether the occurrence of the BDTT near 800^0C is a result of the model or an input to the model. Mobility does influence the strain-rate dependence of T_c, as first observed by St. John (1975), but this should not be taken to indicate that the entire phenomenon is mobility-controlled. Hence, the issue that needs to be resolved is not whether dislocation nucleation or dislocation mobility is the rate-controlling factor but how the two effects can be treated simultaneously in order to obtain a complete description of the phenomenon.

An additional treatment of the problem, as proposed by Gerberich and co-workers (Gerberich *et al.* 1993; Zielinski *et al.* 1992; Huang and Gerberich 1992; Marsh *et al.* 1992; Marsh and Gerberich 1994; Huang and Gerberich 1994), has many features of the mobility-controlled models, but, in fact, assumes that when gliding, dislocations move very rapidly so that they are static during most of the loading time. As in the dynamic models, dislocations are also assumed to be easily generated near the crack tip, according to an initiation criterion, and the dislocation furthest from the tip stops moving when the net local stress drops to the (temperature dependent) CRSS. Fracture is assumed to occur when the local stress intensity at the crack tip (applied K less dislocation shielding) reaches the Griffith value. The variation of fracture toughness with temperature results from changes in the CRSS with temperature, and hence, if the CRSS is approximately temperature-independent around the BDTT, as in many intermetallics, the model does not give meaningful results.

A third point of view is taken in the model developed by one of the principal investigators and his co-workers (Jokl *et al.* 1989; Vitek 1991). This model is based on the assumption that local inelastic deformation necessarily accompanies fracture and that the amount of local plastic deformation is a function of the true surface energy, so that the critical energy release rate i.e. the work to fracture,

$$G_c = 2\gamma + \gamma_p(\gamma) \tag{1}$$

where γ is the true free surface energy of the solid, and $\gamma_p(\gamma)$ is the inelastic work per unit area of crack face, assumed to be a function of γ. This work results from an incipient irreversible shear deformation which occurs simultaneously with the bond breaking and dissipates a significant part of the energy. These shears represent very localized thermodynamically irreversible deformation emanating from the crack tip. They can be described in terms of the motion of 'fractional' dislocations (with Burgers vectors not directly related to the lattice vectors) with very diffuse cores. Further away from the crack tip they may coalesce into usual lattice dislocations. This assertion is based on the fact that if the local tensile stresses at the crack tip are sufficiently large to break atomic bonds, then the shear stresses, which are of the same order of magnitude at the tip as the tensile stress, must be large enough to shear the lattice locally without the need for long range dislocation motion (Jokl *et al.* 1989).

Using this model it has been demonstrated why crack nucleation and subsequent propagation are intrinsically dynamic processes and why the work of fracture associated with extension of microcracks is often more than an order of magnitude larger than the true surface energy. It has been shown (Jokl *et al.* 1989) that a clear distinction needs to be made between pre-existing and injected cracks. While the concomitant bond breaking and thermodynamically irreversible shear deformation (and/or dislocation emission) can take place in the latter case, in the former case any such activity inhibits fracture since it immediately raises the plastic work term to a level exceeding the strain energy release rate. The Rice and Thomson model applies, therefore, in the case of pre-existing cracks.

To summarize the discussion to this point, the onset of quasi-brittle fracture has been viewed either as a result of the competition between local crack extension and dislocation emission or local crack extension and dislocation motion, or as a concomitant process of bond breaking and thermodynamically irreversible shear deformation at the crack tip which directly contribute to the work of fracture (Jokl *et al.* model). In all cases plasticity, albeit very localized, is viewed as absolutely critical to retarding quasi-brittle behavior. Hence, anything that hinders plastic deformation (lower temperature, increasing the yield strength, raising the strain rate, etc.) results in a greater tendency for brittle failure. Consequently, efforts to improve the ductility and toughness of intermetallic compounds, most of which are either brittle or quasi-brittle at low temperatures, have concentrated on increasing dislocation activity in these materials. To date these efforts have not been successful, as is discussed below for Al_3Ti-based intermetallic compounds.

2. Cleavage Failure in $L1_2$ Al_3Ti Based Alloys

The so-called trialuminides of the form Al_3X, where X = Hf, Nb, Ta, Ti, Zr, are of great technological interest because of their low density and high oxidation resistance due to high contents of aluminum. They also tend to have melting temperatures considerably higher than Al, e.g. Al_3Ti melts at 1350°C compared to 660°C for pure Al. Unfortunately they are all very brittle, but their brittleness was initially ascribed to their tetragonal (DO_{22} or DO_{23}) structures. Since these tetragonal structures are expected to have a limited number of slip systems (see e.g. the reviews of Yamaguchi, 1990 and George *et al.* 1991), this brittleness is to be anticipated. However some of these tetragonal structures can be converted to Ll_2 structure by adding ternary alloying elements, e.g. Fe, Cr, and Mn, to Al_3Ti. When Al_3Ti is converted to the $L1_2$ form, a decrease in the flow stress is observed, independent of alloying addition, but the alloy still remains brittle and fails by cleavage. Since the $L1_2$ structure has been commonly thought to be "intrinsically ductile", similar to the case of Ni_3Al single crystals, this brittleness has generated substantial concern in the metallurgical community.

In general the resulting investigations have centered around asking "what is causing this intrinsically ductile material to be brittle?" However, most of the results obtained to date on $L1_2$ Al_3Ti indicate that the material is not at all "intrinsically ductile". It is, in fact, "intrinsically brittle", or, more precisely, "intrinsically quasi-brittle", but the reasons for the brittleness remain obscure. We showed in our previous AFOSR-sponsored program that Al_3Ti has many of the attributes of a normally ductile material–low flow strength, plenty of slip systems — except it is, in fact, brittle. The following are the major results of that research: (#7 comes from parallel research of Kumar, also with AFOSR support).

1. The CRSS for $(111)[\bar{1}01]$ slip is low and is only mildly temperature dependent over a broad range of temperatures between 300 and 1100K but it increases sharply with decreasing temperature below 300K.
2. The CRSS for $(111)[\bar{1}01]$ slip obeys Schmid's law over the entire temperature range.
3. The CRSS for $(111)[\bar{1}01]$ slip is only mildly strain-rate dependent.
4. There is no shortage of slip systems. Slip occurs on all $\{111\} < \bar{1}01 >$ systems and sometimes also on the $\{010\} < 101 >$ system.
5. Substantial compressive ductilities are possible, but no tensile ductility is possible below 1000K.
6. Failure occurs by cleavage on many low index planes.
7. The fracture toughness does not exceed 12 $MPa\sqrt{m}$ at temperatures below 1000K (Kumar 1993).

Based on results #1 - 4, Al_3Ti could be expected to be a reasonably tough material, but we see from results #5 - 7 that it is, in fact, quite brittle (actually quasi-brittle).

Observations #1–7 led to the main idea of the original proposal for this work, *viz*: "the possibility of the production of localized inelastic deformation at the crack tip by processes that do not involve dislocations..." While this idea turned out to be incorrect, it led us to a new model for dislocation generation under the influence of high local stresses.

The work proceeded along two parallel paths: the experimental path in which all possible traditionally-understood reasons for the embrittlement of $L1_2$ Al_3Ti + Fe and Al_3Ti + Cr were explored (and rejected), and the theoretical path, in which dislocation core structure and new dislocation generation mechanisms were investigated. The results of this combined approach are discussed in the next section.

3. Results

3.1 Results — Experimental

In the course of the experiments, a great deal of evidence emerged for the existence of second phase particles, ranging from dramatic differences in CRSS, depending on composition and heat treatment to direct observation the precipitates in optical and electron microscopes. Hence, we concentrated on identifying these precipitates and finding compositions that are single phase $L1_2$ Al_3Ti + Fe or Al_3Ti + Cr. Five different precipitates were identified. While these precipitates further embrittle an already quasi-brittle material, it was concluded that they are NOT the cause of the embrittlement.

Second phase $(Al,Ti)_3Fe$ and Al_3Ti are often seen in compositions containing relatively low Ti contents, such as $Al_{67}Fe_8Ti_{25}$, which lies on the boundary of the nominal single phase $L1_2$ field. The $(Al,Ti)_3Fe$ precipitate has a composition $Al_{66.7}Ti_8Fe_{25.3}$ which is liquid at 1200°C according to (Mazdiyasni *et al.* 1989) The ternary Al_3Ti precipitates which have the DO_{22} structure have composition $Al_{75.6}Ti_{24.0}Fe_{0.4}$, which form clusters scattered throughout the matrix. Although the precipitates seem to be oriented along certain directions in the matrix, there appears to be no orientation relation between the DO_{22} phase and the $L1_2$ matrix.

Computer simulated x-ray diffraction spectra of the DO_{22} Al_3Ti and the $L1_2$ $Al_{267}Fe_8Ti_{25}$ phases have shown that the difference in peak positions is minimum between the {112} plane of the DO_{22} (the Miller indices refer to the tetragonal unit cell of the DO_{22} structure, not to a cubic unit cell, as is commonly done in the literature) and the {111} plane of the $L1_2$. However, even for these two planes, the lattice mismatch is still about 4.5%, which eliminates the possibility of coherent growth of one phase on the other.

The Al_2FeTi (actual composition is $Al_{50.3}Ti_{25.9}Fe_{23.8}$), the so-called T phase, was observed in compounds containing relatively high Fe contents. These precipitates orient randomly in the $L1_2$ matrix of an alloy of composition $Al_{62.5}Fe_{9.5}Ti_{28}$. A similar phase, identified as Al_2NiTi, has been seen in a Ni-modified Al_3Ti alloy (Turner *et al.* 1989).

The Ti_2NAl phase was previously identified to be $Ti_{66.7}Al_{33.3}$, using a conventional SEM (Wu *et al.* 1991; Wu *et al.* 1990). The formation of the $Ti_{66.7}Al_{33.3}$ in the Al-rich matrix was, however, difficult to understand, since it is not consistent with the overall composition of the compounds and was hard to understand based on considerations of the solidification sequence. In addition, the phase is not reported in the high temperature isotherms of the system (Mazdiyasni *et al.* 1989; Markiv *et al.* 1973) It was later found that the phase actually contains N, which was detectable using the SEM but with the beryllium window in front of the x-ray detector removed. An x-ray powder diffraction spectrum and a computer simulation of the spectrum revealed that the phase has a hexagonal structure of the Cr_2CAl-type, with lattice parameters a=2.995Å and c=13.61Å. The Ti_2NAl constitutes a small volume fraction in all the alloys used for the study, but has a large embrittling effect. Cracks are often initiated within the phase or at the interface between the phase and the matrix. Some of the cracks do not seem to have resulted from the mechanical deformation, but probably formed during previous processing and then grew under the applied stress. Moreover, a gap sometimes exists at the interface between the phase and the matrix, indicating a weak bond between the two phases. All these factors contribute to the embrittlement.

Of the five second phases, the Al_2Ti+Fe is probably the most important as far as the structural and mechanical properties are concerned. Based on two-surface trace analysis, the phase forms plates on the cube planes of the $L1_2$ matrix. The volume fraction of the phase depends primarily on Ti-content: the higher the Ti content in the overall composition, the larger the volume fraction of the phase. The phase has a complex tetragonal structure of the Ga_2Hf-type, the same as that of binary Al_2Ti. With small additions of Fe, the a-lattice parameter of Al_2Ti decreases from 3.976Å to 3.95Å, making coherent growth of the precipitates on the cube planes of the matrix possible, since the mismatch between the a-parameter and that of the matrix is then only about 0.3%. The crystallographic relation between the second phase and the $L1_2$ matrix was determined to be $(100)_p//(100)_m$.and $(010)_p//(010)_m$, based on the electron diffraction patterns obtained in the TEM. Because of its complex tetragonal structure, the phase acts as a barrier to the motion of dislocations on the primary octahedral slip planes, the major deformation mode in the $L1_2$ matrix, and results in a strong hardening effect. More detailed discussions can be found in Wu (1992).

In addition to the second phases mentioned above, porosity is also commonly observed. Some of the pores apparently form during interdendritic solidification, while others are probably Kirkendall pores which form in isolated $(Al,Ti)_3Fe$ particles. As has been pointed out by others (Turner *et al.* 1989; Mysko *et al.* 1989), the Kirkendall mechanism might be responsible for the increased void volume fraction seen after a homogenization treatment. The porosity also increases the brittleness of the alloys, providing crack initiation sites leading to premature failure.

In summary, five different second phases, namely, $(Al,Ti)_3Fe$, Al_3Ti, Al_2FeTi, Ti_2NAl and Al_2Ti, have been identified at low temperatures in a number of $L1_2$ Fe-modified Al_3Ti-based alloys, the compositions of which all lie in the nominal single phase $L1_2$ field at 1200°C. Of the five phases, Ti_2NAl and Al_2Ti are probably the most important ones. The former phase exists in virtually all the alloys used for the study and is very deleterious to ductility. The latter forms plate-like precipitates on the cube planes of the $L1_2$ matrix in alloys containing relatively high Ti contents, and has a large hardening effect. In addition to the second phases, porosity also exists and cracks are often seen to initiate at the pores, leading to premature failure. Even though the second phases lead to further embrittlement of $L1_2$ Fe-modified Al_3Ti, the single phase material is, itself, brittle. No second phase is required to initiate cleavage failure.

We then performed some additional experiments to measure the dynamic and static strain aging effects in this material. We measured the stress-strain response in Al_3Ti +Fe as a function of strain, strain rate and temperature and found typical, classical behavior, i.e., the serrations and load drops observed are totally consistent with static and dynamic strain aging effects. We could not, however, identify the solute atom responsible for the effect, but it appears to be a substitutional, not interstitial, atom.

As a result of these experiments we concluded that the brittleness of Al_3Ti is intrinsic to the material. It is not the result of some unknown impurities or second phase particles. This conclusion was very important to the continuation of this research, because it demonstrates that Al_3Ti satisfies all the commonly-stated criteria for high toughness, but it is actually very brittle. These results led to the development of an entirely new model of the Brittle-to-Ductile transition in crystalline materials, which is discussed below.

3.2 Results — Theoretical

3.2.2 A new model for the brittle-to-ductile transition: A cooperative stability

The three principal features which distinguish our approach from the existing models are the following:

(i) *A cooperative dislocation generation instability driven primarily by thermal fluctuations in the presence of an applied stress.*
(ii) An effective thermal-and-stress induced softening of the local medium leading to *screened* dislocation interactions.
(iii) Prediction of the instability based on linear elastic theory of dislocations combined with statistical mechanics description.

The fact that the unstable massive emission of dislocations takes place in a narrow temperature range suggests that the onset of ductile behavior is not a thermally activated phenomenon in the usual sense which takes place in a continuous manner over a wide range of temperatures. The dramatic change in the fracture behavior at the BDT suggests that the phenomenon is a thermally driven instability that results in an enormous increase in the dislocation density.

The notion that thermal fluctuations drive dislocation emission contradicts the traditional thinking in dislocation theory that thermal effects are insufficient to cause spontaneous generation of dislocations (Hull and Bacon 1984). The latter belief stems from the fact that the stress needed to expand a single atomic-size dislocation loop into an unstable configuration is of the order of the theoretical shear strength. The barrier for spontaneous nucleation of dislocations is consequently very high for stresses smaller than the theoretical shear strength, which implies that the probability of generating dislocations is appreciable only if the temperature exceeds the melting temperature. The above conclusion is valid when only one nucleating loop exists, but the situation is quite different when many nucleated loops of different sizes are present at the same time in a medium.

Such a scenario was considered by Kosterlitz and Thouless (K-T) in the context of two-dimensional melting transition (Kosterlitz and Thouless 1973; Young 1979)[1]. They showed that the mutual interactions between the loops (dipoles in two dimensions) gives rise to a *screening effect* which allows a cooperative instability of all the loops to occur at much lower temperatures. This screening is physically distinct from the usual dislocation shielding of the stress field as in the vicinity of the crack tip (Thomson 1986), and does not exist if thermal fluctuations are not taken into account explicitly. In the K-T theory, the unstable emission of dislocations is driven only by thermal fluctuations, without the aid of an applied stress. It occurs close to the melting temperature and causes a dislocation-mediated melting transition (Nelson and Halperin 1979)[2]. In our (two-dimensional) model, both the external stress and thermal fluctuations assist the growth of dislocation dipoles (loops in three dimensions). This causes a K-T type instability to occur well

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[1] The K-T theory represents an important milestone in condensed matter physics and was first proposed in the context of two dimensional (2D) systems with continuous symmetry which do not exhibit a 'conventional' phase transition from a long-range ordered phase at low temperatures to a disordered phase at high temperatures as is the case in three dimensions. Kosterlitz and Thouless showed that a phase transition like behavior nevertheless occurs in such systems and is mediated by topological defects. A well-known example of a topological defect is a dislocation in a crystal characterized by a long-range strain field whereas point defects such as vacancies and interstitials are non-topological in character. An isolated dislocation cannot occur spontaneously at low temperatures in a large system since its energy increases logarithmically with the size of the system. However, defects such as tightly bound dislocation dipoles with separations of dislocations only slightly bigger than the (dislocation) core radius, r_0, have small finite energy. Such configurations represent stable defects that can be formed in the solid by thermal excitations. Thus, at low temperatures, bound dislocation dipoles exist in a crystal but the long range order is not significantly altered by the presence of these defects. However, as the temperature increases, more dipoles with progressively larger separations can be nucleated by thermal activation. At the same time, the population of dipoles of smaller sizes also increases because fluctuations of smaller size are more probable than those of a larger size. A cooperative instability then results above a certain temperature when the mutual interactions between the defects and the gain in entropy make it energetically favorable for the defect pairs to dissociate into isolated defects. A dramatic change in the properties of the system occurs due to the dissociation and proliferation of such topological defects resulting in the destruction of long range order.

[2] Many systems exhibit the K-T type phase transition. Well known examples are (i) melting in two-dimensional crystals caused by the dissociation and proliferation of dislocation dipoles and (ii) the destruction of superfluidity in two-dimensional films due to the dissociation of vortex-pair excitations which interact in a manner completely analogous to dislocations. Recently, the K-T concepts have also been generalized to the case of three dimensional systems in which small topological defects such as dislocation loops in solids and vortex-ring excitations in superfluids exist as stable defects at low temperatures but become unstable above a certain temperature.

below the melting temperature. We begin by explaining the concept of dislocation screening in a qualitative manner.

Dislocation dipoles (or, equivalently loops in three dimensions) with separations (radii) slightly bigger than the (dislocation) core radius, r_0, have energies of the order of 1-2 eV. Hence, such atomic configurations represent metastable defects that can be nucleated by thermal agitations at finite temperatures in all solids (Kosterlitz and Thouless 1973). The existence of a certain (thermal) fluctuation which leads to the formation of a dipole of size r automatically implies that dipoles of size smaller than r exist with higher probability. Thus a loaded elastic solid at finite temperatures contains a certain concentration of dislocation dipoles (loops) of different sizes.

The creation of each dipole (loop) by thermal fluctuations induces in the medium a certain amount of plastic strain in addition to the elastic strain. The interaction between the dipoles (loops) and the coupling of the dislocation fields with the applied traction (the latter is equivalent to the microscopic work done by the applied stresses in nucleating the dipole) can be taken into account if the response of the medium to the applied stress is measured in terms of the total strain, as opposed to the purely elastic strain, giving rise to an "effective shear modulus". This definition can be used to write the total energy of the system (including interactions and couplings) as a sum of reduced self energy of the dislocation dipoles (loops) and reduced elastic energy of the solid expressed in terms of the effective (or, renormalized) moduli (Nelson and Halperin 1979). A simple way to visualize the interaction effect is to invoke the analogy of bound electric dipoles in a dielectric medium inducing polarization which leads to screened self-interactions (Kosterlitz and Thouless 1973). In the present context, a larger dislocation dipole is screened by the smaller dipoles present in the medium which in effect lowers the self energy of the large dipole. This apparent change in the local properties enables more dipoles to be nucleated by thermal activation causing a cumulative effect. Thus the creation of many atomic-size dipoles (loops) induces a temperature-dependent *cooperative screening effect* that enhances the subsequent growth of the dipoles (loops) with increase in temperature and/or stress.

A thermally-induced instability occurs above a certain temperature for a given stress level σ, when it becomes energetically favorable to dissociate the dipoles resulting in a rapid increase of 'free' dislocations[3]. The onset of the dislocation emission instability can be studied by investigating the behavior of the effective shear modulus using standard techniques of statistical mechanics (Kosterlitz and Thouless 1973; Khanta *et al.* 1994). The latter serves as a good probe to distinguish between the elastic and plastic response since the effective modulus vanishes when the dipoles dissociate (or, equivalently when the loops attain a critical radius) and plastic flow begins. The screening of a test dipole of separation r by all dipoles of separation less than r can be expressed via a scale-dependent polarizability $\varepsilon(r)$. It can be shown (Khanta *et al.* 1994) that the divergence of the polarizability, corresponding to a rapidly increasing 'free' dislocation density, occurs at a temperature

$$T_c = \frac{1}{2k_B}\left(\frac{q^2}{\varepsilon(r_c)} - \frac{\sigma b r_c}{2}\right) \tag{2}$$

where $q^2 = (\mu_0 B_0/(\mu_0+B_0))b^2/2\pi = (\mu_0/(1-\nu))b^2/4\pi$, μ_0 and B_0 are two-dimensional shear and bulk moduli in the absence of dislocations (expressed in units of N/m), ν represents Poisson's ratio, b is the Burgers vector of the dislocation, k_B is the Boltzmann constant and r_c is the critical radius for the dissociation of the dipole.

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[3] It should be emphasized that while the nucleation of small dislocation dipoles (loops) is thermally activated the onset of the dissociation instability is a purely cooperative effect which occurs sharply at a certain temperature.

This expression for T_c is actually derived as an unstable fixed-point of a set of nonlinear equations describing the dependence of $\varepsilon(r_c)$ on T and σ.

Equation (2) gives the temperature at which a sudden extensive generation of dislocations occurs in an initially dislocation-free material subjected to a certain stress. Hence, it either determines the stress at which a sudden avalanche of plastic deformation occurs at a given temperature or it determines the temperature at which the massive plastic deformation sets forth at a given stress. In the context of the BDT, the initial sample contains a sharp crack and the interpretation of the above equation is as follows: Let us assume that the local stress near the crack tip (which is the preferred site for dislocation emission) attains the value at which the Griffith-like criterion for brittle crack propagation is satisfied. When the stress in equation (2) corresponds to this situation, T_c is then expressed only in terms of material parameters. For temperatures lower than T_c, the dislocation emission instability does not occur and, instead, crack propagation takes place. At T_c a massive amount of dislocation generation occurs at this stress level which completely precludes crack propagation. Thus, T_c corresponds to the BDTT which signals the onset of ductile behavior.

A linear stability analysis carried out (Khantha *et al.* 1994) around the fixed point along with the initial conditions for the nonlinear equations allows one to express T_c as a function of material parameters including the dislocation core radius and energy. The reason that the parameters which determine T_c are not, in principal, different from those occurring in the Rice-Thomson model (Rice and Thomson 1974; Rice 1992) and even other previous models (Armstrong 1966; Kelly *et al.* 1967) lies in the fact that these quantities define the energy of a dislocation in a theory based on linear elasticity, which forms a common starting point of all the models. However, our approach includes the local changes (e.g., shear softening) of the surrounding medium due to the creation and interaction with other dislocations. This feature makes our model far less sensitive to the precise values of the core parameters since the cooperative interaction is averaged over all statistically possible configurations unlike the earlier approaches which rely entirely on the geometry of a single dislocation. Nevertheless, it is possible to recover the single dislocation result by going to the limit of zero transition temperature, when dislocation screening is absent, i.e., $\varepsilon(r_c) = 1$. Equation (2) reduces to the well known criterion for homogeneous nucleation: $\sigma = (\mu_0 b/2\pi(1-\nu)r_c)$. The Rice-Thomson result for spontaneous dislocation emission in two dimensions (Rice and Thomson 1974) can be obtained by equating this critical stress to the local stress at a distance r_c from the tip assuming the fracture load to be given by the Griffith threshold.

The importance of the thermally induced dislocation screening effects is seen by calculating the BDTT from equation (2) using the same values of the material parameters as in the Rice-Thomson model (Rice and Thomson 1974). For typical values of the surface energy of brittle materials, the local stress at a distance r_0 from the crack tip is of the order of $\mu_0/10$. For Si, our approach predicts $T_c \sim 1000$ K, whereas the zero-temperature Rice-Thomson result (Rice and Thomson 1974) predicts an activation barrier of 111eV which is equivalent to $T_c \sim 10^6$ K[4]. For W, we obtain T_c equal to ~ 3000 K, while the Rice-Thomson result for the activation barrier in this case is 329eV which is equivalent to $T_c \sim 3\times10^6$ K. Our results are in good qualitative agreement with observations considering the fact that the model does not take into account the presence of pre-existing free dislocations. T_c is, indeed, typically two-thirds of the melting temperature for very brittle materials. In its present form the model cannot be used for systems in which the initial dislocation density is large, as this would be contrary to the assumptions made in developing the theory. Nevertheless, if we (unrealistically) apply the model to Cu (which is

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[4] The activation barrier for the case of Si has been re-stimated by Haasen and more recently by Rice to be less than 1eV. If this is true, spontaneous generation of dislocations should be possible even at room temperature but the experiments clearly show that this is not the case.

f.c.c. and does not undergo a BDT), we obtain T_c = 10K with r_0~b i.e., the transition temperature is very low, a small fraction of the melting temperature. The obvious correlation between the transition temperature and quantities such as the Burgers vector, the shear modulus, etc., come out of the model in a straightforward manner. The calculations based on this simple model clearly demonstrate that the thermally-induced dislocation screening plays an important role in the BDT and, in fact, causes its strong temperature dependent character.

4. Conclusions

Based on the results of our combined experimental/theoretical research on $L1_2$ Al_3Ti + Fe and Al_3Ti + Cr we conclude the following.

1. Many brittle precipitates form in Al_3Ti + Fe which can serve as preferred crack paths.
2. However, even without these precipitates $L1_2$ Al_3Ti cleaves, and therefore Al_3Ti + Fe and Al_3Ti + Cr with the $L1_2$ crystal structure are inherently quasi-brittle.
3. We have formulated a new model for the BDT based on a temperature-driven, stress-assisted dislocation instability. In this model at the BDT the combination of stress and temperature cause a divergence in the dislocation density, even in the absence of pre-existing dislocation sources.

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Mechanisms of Quasi-Brittle Failure in Metals and Intermetallic Compounds

Post-doctoral fellows and graduate students participating in program

Post-Docs and Research Associates

Mahadevan Khantha
Zilu Wu

Graduate Students

Robert Folk
Steven Gradess

List of Publications

Z.L. Wu and D.P. Pope: "The Deformation and Fracture of Single Crystalline L1$_2$Al$_3$ Ti + X Alloys", in *Structural Intermetallics*, edited by R. Darolia, J.J. Lewandowski, C.T. Liu, P.L. Martin, D.B. Miracle and M.V. Nathal, TMS, Warrendale, PA (1993), pp. 107-116.

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