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13. ABSTRACT (Maximum 200 words)

State-of-the-art first-principles electronic structure calculations based on the *full-potential linear-muffin-tin-orbital* method and the pseudopotential method were employed to study systematically: 1) The electronic structure of the "clean" tilt $\Sigma 5$ grain boundary in Ni_3Al ; 2) The effect of hydrogen on the $\Sigma 5$ grain boundary in Ni_3Al ; 3) The generalized stacking fault energy surface and dislocation properties of aluminum; 4) The correlation of the topology of the electronic charge density with the energetics and stability of planar faults in fcc metals; ~~5) The grain boundary sliding and the effect of vacancy on the grain boundary migration;~~ 6) The unusual magnetic properties of the Cerium mononictides and monochalcogenides; and 7) The ground-state properties of the one-dimensional Hubbard model at half-filling in the presence of a magnetic field.

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**ELECTRONIC STRUCTURE AND MECHANICAL
PROPERTIES OF INTERMETALLICS**

FINAL PROGRESS REPORT

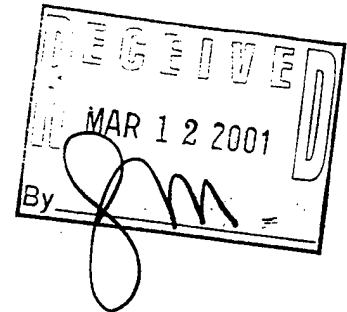
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State-of-the-art first-principles electronic structure calculations based on the *full-potential* linear-muffin-tin-orbital method and the pseudopotential method were employed to study systematically: 1) The electronic structure of the "clean" tilt $\Sigma 5$ grain boundary in Ni_3Al ; 2) The effect of hydrogen on the $\Sigma 5$ grain boundary in Ni_3Al ; 3) The generalized stacking fault energy surface and dislocation properties of aluminum; 4) The correlation of the topology of the electronic charge density with the energetics and stability of planar faults in fcc metals; 5) The grain boundary sliding and the effect of vacancy on the grain boundary migration; 6) The unusual magnetic properties of the Cerium monopnictides and monochalcogenides; and 7) The ground-state properties of the one-dimensional Hubbard model at half-filling in the presence of a magnetic field.

FINAL PROGRESS REPORT

I. Statement of the problem studied

We have carried out theoretical studies of the electronic structure and mechanical properties of the $L1_2$ -type ordered nickel-based intermetallics and of the fcc metals (Al, Ag), exhibiting unique mechanical properties that make them attractive for aerospace and U.S. Army applications at elevated temperatures. This research work was supported by a U.S. Army grant (DAAG55-97-1-0093) in the amount of \$179,319 from 03/96 to 02/2000. The immediate motivation of this research work is the unusual mechanical properties of this class of intermetallics (high melting temperature, low density, increase of yield stress with increasing temperature, good oxidation resistance), their importance in designing new ductile ordered superalloys, and the need for a better understanding of the electronic and mechanical properties at the atomistic level.

A major part of our effort focused on applying state-of-the-art first principles electronic structure calculations to study systematically:

1. The electronic structure of the "clean" tilt $\Sigma 5$ grain boundary in Ni_3Al ;
2. The effect of hydrogen on the $\Sigma 5$ grain boundary in Ni_3Al ;
3. The generalized stacking fault energy surface and dislocation properties of aluminum;
4. The correlation of the topology of the electronic charge density with the energetics and stability of planar faults in fcc metals;
5. The grain boundary sliding and the effect of vacancy on the grain boundary migration;
6. The unusual magnetic properties of the Cerium monpnictides and monochalcogenides; and
7. The ground-state properties of the one-dimensional Hubbard model at half-filling in the presence of a magnetic field. This last research project was supported 30% from the US Army Grant and 75% with matching funds from California State University Northridge.

These microscopic quantum mechanical calculations are based on the full-potential Linear-Muffin-Tin-Orbital (FPLMTO) method and the pseudopotential method and include structural relaxations. The full potential capability is essential when dealing with intermetallic compounds, which combine those characteristics common to covalently bound materials with metallic properties – a fairly uncommon combination. On the other hand, the pseudopotential calculations allow the treatment of a larger number of atoms in the supercell. In contrast to atomistic simulations based on empirical potentials or the embedded-atom method involving the process of fitting parameters, first principles electronic structure calculations provide insight into the chemical bonding characteristics which ensue the cohesiveness of interatomic forces that control mechanical properties, and allow the possibility of not only studying "clean" intermetallics, but also intermetallics containing chemically different impurities.

The publications resulted from this research work are listed as Refs. 1-17 in the Bibliography. In Sec. II, we present the summary of the most important results. The list of publications resulted from this research work during the 1996-2000 period is presented in Sec. III. The scientific personnel involved in the research work are listed in Sec. IV. The Computational Materials Theory facilities are listed in Sec. V. The bibliography is presented in Sec. VI.

II. Summary of the most important results

1. Electronic structure of the "Clean" tilt grain boundary in Ni_3Al

As with many intermetallics, an inherent drawback to using Ni_3Al as a structural material is the tendency of polycrystalline ordered stoichiometric alloys to undergo brittle intergranular fracture, even though single crystals of Ni_3Al are highly ductile.¹⁸ This propensity towards intergranular fracture is traced to the reduced cohesion between adjacent grains at their shared grain boundaries, particularly to the structural and atomic compositional details at these grain boundaries, including various impurities that diffuse and segregate in these domains from the bulk.¹⁹

We have applied *ab initio* electronic structure calculations to investigate the electronic origin which is responsible for such characteristic grain boundary properties.^{5,8,10} The purpose of this work was to gain insight on how the local environment at the grain boundary changes the bonding charge distribution from that in the bulk. We have shown that the bonding charge distribution in the boundary region is different from that in the bulk due to the different atomic arrangement (bond defects).²⁰ In general, the charge across the grain boundary is reduced. The redistribution of bonding charge could potentially modify the crack propagation characteristics along the boundary in Ni₃Al. We have calculated the interlayer strain perpendicular to the grain boundary which shows an oscillatory behavior with a rapidly decaying profile with increasing distance from the boundary plane. We have shown that there is a *rippling effect* between the Al and Ni atoms in the vicinity of the interface, and a strong electrostatic repulsion between the Al-Al atoms due to the depletion of bonding charge at the Al site. Thus, replacement of these Al atoms by Ni atoms would lead to an increased cohesion between the two grains. This is consistent with the experimental results that the Ni-rich boundary is more resistant to intergranular fracture.^{21,22} We have calculated also the excess grain boundary expansion, the grain boundary energy, and the Griffith energy.

2. Effect of Hydrogen on the Grain Boundary in Ni₃Al

While the *intrinsic* factors, such as poor grain boundary cohesion, are important, in many cases dominant, in limiting ductility, recent work by George *et al* has shown²³ that *extrinsic* factors, in particular the humidity, can be a major cause of low ductility in some systems. Their results demonstrate that the poor ductility commonly observed in air tests involves the dissociation of H₂O to generate atomic hydrogen, which diffuses into the region of the crack tip and promotes brittle crack propagation. George *et al*²³ have suggested that the principal role of boron in ductilizing Ni₃Al is to suppress the environmental embrittlement.

We have studied^{3,8,10} the effect of local environment of the hydrogen impurity on the electronic structure by placing the impurity at two different interstitial sites: a) on the Ni-Al mixed (001) plane and b) on the pure Ni (002) plane. Hydrogen prefers to occupy interstitial sites on the Ni-rich boundary planes. Hydrogen is found to reduce in general the bonding between the Ni atoms across the grain boundary and to enhance the bonding-charge directionality of the Ni atoms at grain boundary. This suggests that hydrogen reduces the local grain boundary cohesion. We have employed Rice's thermodynamic model²⁴ to examine the energetics of the hydrogen induced-weakening of the grain boundary cohesion. The positive difference in formation energy for hydrogen at the grain boundary and at the free surface of 1.4 eV, indicates the embrittling potency of hydrogen in the Ni₃Al grain boundary. Overall, we find that our calculations are in agreement with the known behavior of hydrogen in Ni₃Al,²³ and they provide insight into the bonding behavior underlying the weakening of the grain boundary cohesion.

3. Generalized Stacking Fault Energies and Dislocation properties of Aluminum

There has been a great deal of interest in describing accurately the dislocation core structure on an atomic scale because of its important role in many phenomena of crystal plasticity.^{25,26} The core properties control, for instance, the mobility of dislocations, which accounts for the intrinsic ductility or brittleness of solids. Two types of theoretical approaches have been employed to study the core properties of dislocations. The first type is based on direct atomistic simulations employing either empirical potentials or first principles calculations. Empirical interatomic potentials involve the fitting of parameters to a predetermined database and hence may be not reliable in describing the core properties, where severe distortions like bond breaking, bond formation and switching necessitate a quantum mechanical description of the electronic degrees of freedom. On the other hand, first-principles electronic structure calculations, though considerable more accurate, are computationally expensive for studies of dislocation properties. The second type of approach is based on the framework of the Peierls-Nabarro (PN) model which seems to be a plausible alternative to direct atomistic simulations. In fact, there has been a resurgence of interest in the simple and tractable P-N model for the study of dislocation core structure and mobility.^{27,28}

This research work was carried out in collaboration with Dr. Vasily Bulatov at Lawrence Livermore National Laboratory and Prof. Efthimios Kaxiras at Harvard University. We have employed¹² the recently developed semidiscrete variational generalized PN model²⁹ to study for the first time the dislocation core properties of aluminum, which is prototypical ductile metal with much lower Peierls energy and stress than silicon. On the other hand, just like silicon, aluminum is known to have a narrow core due to its large stacking fault energy. The generalized stacking fault energy surface entering the model is calculated from first principles electronic structure calculations and the embedded atom method (EAM). The EAM can give gross trends for various dislocation properties but fails to predict the finer core structures, which in turn can affect the Peierls stress significantly. We have investigated various core properties, including the core width, splitting behavior, energetics and Peierls stress for different dislocations. Our results reveal a simple relationship between the Peierls stress and the ratio between the core width and atomic spacing. The successful application of the new model to aluminum further proves its validity and versatility in predicting dislocation core properties of different materials.

We have reexamined also two essential issues within the Peierls-Nabarro model which are critical in obtaining accurate values for the Peierls stress.¹⁶ The first issue is related to the **sampling scheme of the misfit energy across the glide plane and the second one is the effect of relaxation on the Peierls stress.** We have shown that most of the current applications of the Peierls-Nabarro model do not treat properly the two issues and therefore are not able to predict reliable values for the Peierls stress. The double counting scheme for the misfit energy at both sides of the glide plane was found to be **physically more reasonable, and to predict more accurate values for the Peierls stress, especially for dislocations with equal spacing between alternating atomic rows.**

Finally, our results demonstrate the importance for allowing relaxation when a dislocation traverses the Peierls barrier, which in turn lowers the Peierls stress for narrow dislocations by an order of magnitude. In the next stage, we will apply the new model in intermetallics, where no results are available.

4. Correlation of Topology of Charge Density with the Energy and Stability of Planar Faults in Metals

The competition between ductile and brittle behavior is of importance in the design of products using metallic components. For ductile failure occurs over many cycles of operation, whereas brittle failure often occurs suddenly with catastrophic results. An explanation for the susceptibility of a material to cleavage could be determined by a straightforward assessment of the relative strengths of bonds across the cleavage plane to those across slip plane.³⁰ The purpose of this work was to investigate the correlation of the energetics associated with the shear deformation in fcc metals (Al and Ag) and the evolution of the topology of the electronic charge density. During the shear process where a bond is broken, the extra charge located in the metal bond being broken must be redistributed. The redistribution of this charge will depend on the local environment, which can either accommodate this charge in the existing unbroken bonds or not.³¹

Since our work in this area will be submitted shortly to Physical Review B,¹⁷ we describe some of the results here. We have studied two prototypical ductile metals, Al and Ag, which have quite different deformation properties. The intrinsic stacking fault energy in aluminum (166 mJ/m^2) is about five times larger than that of silver (30 mJ/m^2). The value of the intrinsic stacking fault energy dictates the dissociation of full dislocations and the separation between the partials. The EAM potential, used very often to study mechanical properties in metals (crack propagation, etc.) underestimates the intrinsic stacking fault energy by a factor of two.¹² This indicates the importance of using full potential electronic structure calculations (FPLMTO) which provide not only accurate energetics but also information on the topology of the charge density responsible for the rearrangement of bonds. The *ab initio* calculated intrinsic stacking fault energies are in excellent agreement with experiment. We find that the slip process occurs earlier (50% of the shear displacement) for Ag and later (63% of the shear displacement) for Al. The unstable stacking fault energy is 219 mJ/m^2 and 195 mJ/m^2 for Al and Ag, respectively.

We have calculated the evolution of the charge density in a plane perpendicular to the bond direction between a pair of A-C atoms across the shear (111) plane as the A-C bond {\it \it forms}, for both Al and Ag. At zero shear, the curvatures along and perpendicular to the bond direction of the breaking AC bond in Ag are about an order of magnitude larger than the corresponding ones in Al. On the other hand, at zero shear the curvatures for the forming bond are similar for both Al and Ag. During the shear process we find the following interesting and important results. Note, that at the position where the energy reaches its maximum value, at least one of the two curvatures perpendicular to the bond vanishes (signaling a topological instability). More specifically, for Ag both curvatures perpendicular to the bond vanish at the unstable stacking fault energy, whereas for Al only one goes to zero at the unstable stacking fault energy whereas the other vanishes very close to the intrinsic stacking fault energy. These results indicate that the bond breaking and bond forming processes for Ag are accommodated with an *easier* redistribution of charge. In fact, the topology of the charge density for Ag at the intrinsic stacking fault energy is very similar to the unsheared bulk configuration. This explains the fact that the intrinsic stacking fault energy of Ag is five times smaller than that for Al. On the other hand, the charge density of Al for the intrinsic stacking fault configuration resembles that for the **unstable stacking fault configuration and hence the corresponding energies are quite similar. The fact that the bonds of Ag respond to the shear strain in an electrophilic manner is closely related to the fact that Ag has only s orbitals while Al has both 3s and 3p contributing to the bonding (the p orbitals of Al are more directional).**

5. Grain boundary sliding in metals

It is well established that grain boundaries play an important role in the behavior of materials, particularly in its inelastic response as well as fast self-diffusion mechanism along the plane of the interface.^{32,33} The most pronounced structural feature of a grain boundary is the atomic-level disorder near the interface even at zero temperature.³⁴ The fact that structural properties at or near the interface can differ dramatically from those of the surrounded bulk material determines its inelastic response. Rigid body translation parallel to the interface strongly affects the atomic structure along the interface and plays an important role in the deformation process providing plastic shear displacements, i.e. superplastic flow. Two principal mechanisms of plastic flow at intermediate-to-high temperatures are grain boundary sliding and diffusional flow.³⁵ Computer simulations offer the unique ability to examine the details of the grain boundary sliding under the application of external stress.

While *ab initio* electronic structure calculations provide accurate structural information and energetics, they are limited to a small ensemble of atoms. We have employed¹³ finite-temperature Monte Carlo simulations based on the embedded atom method (EAM) potential, to study the microscopic mechanism for sliding of the $\Sigma 5$ grain boundary in aluminum. We used the simulated annealing technique to obtain the optimal configuration. We find that the grain-boundary (GB) energy changes *discontinuously* at certain sliding distances which are associated with the grain-boundary *migration*, defined as the motion of the interface in the direction perpendicular to the boundary plane. The mobility of the GB migration is found to depend on the annealing temperature. Analysis of the atomic structure reveals that the migration is **mediated by the thermally activated flow of the atoms along the interface in coordination with the atoms in the bulk.** We are currently submitting a manuscript to Physical Review B.

We have also investigated the effect of vacancies on the grain boundary sliding. Grain boundaries provide pathways for diffusion into or within a material that can be orders of magnitude faster than through crystalline regions. There have been suggestions that the energy formation of vacancies will be lower in the grain boundary or in the surface region than in the bulk. However, no experimental evidence is available to approximately quantify the extent of these effects. Because the atomic environment around a point defect is very different from the bulk, a consistent description of all the defect properties seems to require some sort of explicit treatment of the electronic degrees of freedom.

We have applied *ab initio* electronic structure to investigate the electronic origin of the effect of a vacancy on the grain boundary sliding of the S5 tilt grain boundary in Al.¹³ In order to gain a full understanding of the interaction of the vacancy with the grain boundary, we have placed the vacancy at various possible atomic sites. Our results show that the vacancy formation energy depends on the local atomic environment of the vacancy. More specifically, we find that the vacancy formation energy is higher than its bulk value (0.1 eV) when the vacancy is placed at the grain boundary plane, and is much lower (0.23 eV) than the bulk value when the vacancy is at the first layer to the boundary. These results indicate that the grain boundary does not always act as a sink of vacancies. Rather, vacancies migrate selectively to planes adjacent to the boundary. Another important finding is that the atomic relaxation induced by the vacancy is larger than that due to the grain boundary (GB expansion). We have calculated also the energy profile during sliding in the presence of a vacancy. Interestingly, we find that the vacancy increases the sliding energy barrier by a factor of about three compared to that for the pure GB, and it eliminates completely grain boundary migration. The inhibition of one mode of GB motion and GB migration by a single vacancy, is similar to the dragging effect for dislocation motion induced by a point defect atmosphere. These results suggest that creation of vacancies at GB may improve the high temperature stability of polycrystalline materials, just as the common practice of solute strengthening in alloys. Two manuscripts are currently under preparation for submission to Physical Review B.¹³

6. Magnetic properties of Strongly Correlated Electron Systems

The isostructural (rock-salt structure) series of the cerium monopnictides CeX (X = P, As, Sb, Bi) and monochalcogenides (X=S, Se, Te) have become prototype model systems for study, because of their unusual magnetic properties.³⁶⁻³⁷ This series of strongly correlated electron systems offers the opportunity to vary systematically, through chemical pressure, the lattice constant and the cerium-cerium separation on going down the pnictogen or chalcogen column, and hence tailor the degree of 4f localization from the strongly correlated limit in the heavier systems to the weakly correlated limit in the lighter systems. The sensitivity of the hybridization, Coulomb exchange, and crystal-field interactions to the chemical environment gives rise to a variety of unusual magnetic properties. This class of cerium systems exhibits large magnetic anisotropy which changes from the <001> direction in the pnictides to the <111> direction in the chalcogenides. The low temperature magnetic moment increases with increasing lattice constant for the pnictides from 0.80 μ_B in CeP to 2.1 μ_B in CeSb and CeBi, while it decreases with increasing lattice constant for the chalcogenides from 0.57 μ_B in CeS to 0.3 μ_B in CeTe.³⁶⁻³⁷ The magnetic moment collapse from CeSb to CeTe, with both systems having about the same lattice constant, is indicative of the sensitivity of the exchange interactions to chemical environment.

The purpose of this work is to apply two *ab initio* based methods to investigate the origin in the electronic structure of the unusual magnetism across this series of compounds.¹⁵ Comparison of the two methods will test the limitations of the two *ab initio* based calculations as the degree of 4f localization is varied across the series, and will reveal the failure of standard *ab initio* electronic structure calculations, based on density functional theory within the local density approximation (LDA), to predict, even qualitatively, the trend of magnetic properties in this series of strongly correlated electron systems. The second *ab initio* based method gives clear insight on the interplay of the exchange and crystal field interactions, and gives results for the magnetic moments, magnetic structure, and ordering temperatures in excellent agreement with experiment. The first method employs standard *ab initio* spin polarized electronic structure calculations based on the full potential linear muffin tin orbital (FPLMTO) method using 1) only spin polarization, with the orbital polarization included only through the spin-orbit coupling, and 2) both the spin and orbital polarization. In these calculations the 4f states are treated as band states. The second *ab initio* based method employs the degenerate Anderson lattice model, which incorporates explicitly the hybridization and the Coulomb exchange interactions on an equal footing. The parameters entering the model Hamiltonian are evaluated on a wholly *ab initio* basis from FPLMTO calculations.

We have calculated the zero-temperature cerium magnetic moment from FPLMTO electronic structure calculations both with and without the orbital polarization correction taken into account. As expected, in all cases, the orbital polarization is found to be opposite to the spin polarization. Comparison of the total energies gives that the magnetic anisotropy changes from the $\langle 001 \rangle$ direction in the pnictides to the $\langle 111 \rangle$ in the chalcogenides, in agreement with experiment. On the other hand, except perhaps for the lighter chalcogenides (CeS and CeSe), comparison of the *ab initio* and experimental values for the magnetic moment indicates the *failure* of the LDA calculations to treat properly the correlation effects of the 4f states (treated as band states) within the LDA as the degree of 4f correlations increases in the heavier pnictide systems. Furthermore, the *ab initio* calculations fail to predict the large moment collapse from CeSb to CeTe, the latter being described as an incipient heavy Fermion system.

Overall, we find that the second *ab initio* based approach which takes into account all three pertinent interactions (hybridization, Coulomb exchange, and CF interactions) on an equal footing, yields results for both the zero-temperature moment and the ordered temperature (a more stringent test for the theory) in excellent agreement with experiment. A final corroboration of the success of the second *ab initio* based method is that it predicts the experimentally observed change of the ground-state magnetic structure from the $\langle 001 \rangle$ antiferromagnetic type IA ($\uparrow\uparrow\downarrow\downarrow$) in CeBi and CeSb to the $\langle 001 \rangle$ antiferromagnetic type I ($\uparrow\downarrow$) in CeAs and CeP.³⁶⁻³⁷

7. Magnetic crossover in the one-dimensional Hubbard model in the presence of magnetic field

This research project was supported 25% from the US Army Grant and 75% from California State University Northridge. The repulsive Hubbard model is the simplest model that includes the basic ingredients of electron correlations for the treatment of the metal-insulator transition and magnetism.^{38,39} The model displays the many-body physics responsible for the interplay between the Mott-Hubbard localization and antiferromagnetism, and is currently a subject of intensive study due to its possible relevance in high Tc superconductivity.⁴⁰

The purpose of this work¹⁴ was to apply a generalized mean-field (GMF) treatment, which includes both the spin-density and the antiferromagnetic ordering in the x-y plane on an equal footing, to study the ground-state properties of the Hubbard model in the presence of magnetic field, and to compare the GMF results with the Bethe-ansatz solutions.⁴¹ We find that the ground-state energy, the magnetization, the effective kinetic energy and the number of double occupied sites are in qualitative, and in some case, quantitative agreement with the exact results over a wide range of interaction parameters. The good agreement between our results and the exact ones in one dimension puts the GMF approach on firmer basis in two and three dimensions, where the effect of fluctuations is weaker. The calculated phase diagram exhibits a magnetic crossover from itinerant electron-hole pairs to a Bose-Einstein condensated state of local pairs.¹⁴ Work currently in progress is aimed at applying the GMF approach to generalized versions of Hubbard-like models and to higher dimensions, where exact results are lacking.

III. Publications

1. *Chemical Bonding and Elastic Constants of Nickel-Based Intermetallics*, N. Kioussis, J. Blanco, S. P. Lim, and R. Wu, in *Properties of Complex Inorganic Solids*, eds. A. Gonis, A. Meike, and P. Turchi, 389 (Plenum, New York, 1997).
2. *First principles determination of hyperfine fields in Pt/Fe (111) multilayers*, G. Lu, R. Wu, L. Chen, and N. Kioussis. NATO ASI *Magnetic Hysteresis in Novel Magnetic Materials*, Series E. **338**, 179 (1997).
3. *Ab initio electronic structure of the $\Sigma 5$ Grain Boundary in Ni₃Al*, G. Lu and N. Kioussis, Mater. Res. Soc. Symp. Proc. **472**, (1997).

4. *First principles investigations of 4d magnetism on C(0001)*. L. J. Chen, R. Wu, N. Kioussis, and J. Blanco, *J. Appl. Phys.* **81**, 4161 (1997).
5. *Electronic mechanism of oxygen embrittlement of TiAl*. Y. Liu, K.Y. Chen, J. H. Zhang, Z. Q. Hu, G. Lu, and N. Kioussis, *J. Phys. Cond. Matter. Phys.* **9**, 9829 (1997).
6. *One-dimensional Hubbard Model in the presence of magnetic field*. N. Kioussis, A. Kocharian, and S. Park. *J. Magn. Magn. Mater.* **177-181**, 575 (1997).
7. *First principles determination of the bonding mechanism and adsorption energy for CO/MgO (001)*. L. Chen, R. Wu, N. Kioussis, and Q. Zhang. *Chem. Phys. Lett.* **290**, (1998).
8. *First principles studies of the $\Sigma 5$ tilt grain boundary in Ni₃Al*. G. Lu, N. Kioussis, R. Wu, and M. Ciftan, *Phys. Rev. B* **59**, 891 (1999).
9. *Ab initio study of anisotropic magnetism in Uranium compounds*, E. Collins, N. Kioussis, and S. P. Lim, *J. Appl. Phys.* **85**, 6226 (1999).
10. *Effect of hydrogen on grain-boundary embrittlement: An ab initio study*, G. Lu, N. Kioussis, R. Wu, and M. Ciftan, in *Condensed Matter Theories*, **15**, (Nova, Spring 2000, in press).
11. *Tight-binding study of stacking faults and the Rice criterion of ductility in the fcc metals*, M. Mehl, D. Papaconstantopoulos, N. Kioussis, and M. Herbranson, *Phys. Rev. B* **61**, 4894 (2000).
12. *Generalized stacking fault energy surfaces and dislocation properties of Aluminum*, G. Lu, N. Kioussis, V. Bulatov, and E. Kaxiras, *Phys. Rev. B* **62**, 3099 (2000).
13. *Monte Carlo simulations of grain boundary sliding: Effect of vacancies*, P. Ballo, N. Kioussis, and G. Lu, to be submitted to *J. Mater. Research* (2000); *Effect of a vacancy on grain boundary sliding*, G. Lu and N. Kioussis, submitted to *Phys. Rev. B* (2000).
14. *Development of Magnetism in Strongly Correlated Electron Systems: Non-Kondo mechanism for moment collapse*. E. Collins, N. Kioussis, S. P. Lim, and B. R. Cooper, *Phys. Rev. B* **62**, 11533 (2000).
15. *Interplay between crystal field and exchange interactions in strongly correlated Cerium systems*, E. Collins, N. Kioussis, S. P. Lim, and B. R. Cooper, *J. Appl. Phys.* **87**, 5143 (2000).
16. *The Peierls-Nabarro model revisited*. G. Lu, N. Kioussis, V. Bulatov, and E. Kaxiras, *Phil. Mag. Lett.* **80**, 675 (2000).
17. *Correlation of topology of charge density and stability of planar faults in metals*, N. Kioussis, M. Herbranson, and M. Eberhart, to be submitted to *Phys. Rev. B* (2000).

IV. Participants and scientific personnel

The U.S. Army grant award has aided our development of a strong research program in the area of Theoretical Condensed Matter Physics at California State University Northridge (CSUN). The program has provided undergraduate and graduate students the opportunity to get hands-on experience with active researchers and to build a solid foundation for further scientific study and research careers. Students attend seminars that have grown out of the research program and participate in research via projects in upper level Solid State courses. A new graduate course,

Advanced Topics in Solid State. has been added to the curriculum to introduce students to topics such as density functional theory, correlated electron systems, computational materials science, etc.

Seven students have been involved in the research program over the past four years and have been supported by external (NSF and US Army) and internal grant awards. Two of these students (Mr. G. Lu and Mr. E. Collins) have earned the Ph.D. degree and two (Ms. M. Herbranson and Mr. S.H. Park) have earned the M.S. degree. Mr. S. H. Park has continued his graduate studies at the University of Chicago. A fifth graduate student, Mr. H. Scudder, is working on his MS thesis, to be completed in Summer, 2001. Dr. Gang Lu (a post-doctoral fellow) and Dr. Armen Kocharian were supported by U.S. Army and matching CSUN grants. The U.S. Army Augmentation Award for Science and Engineering Research Training (1995-1999) has also provided support to three graduate students, Ms. M. Herbranson, H. Scudder, and E. Collins (Ph. D. student), and to two undergraduate students, Mr. J. Pruet and Mr. J. Noland. Mr. J. Pruet has continued his Ph.D. studies at Yale. Collaboration with Harvard University (Prof. E. Kaxiras), MIT (Dr. V. Bulatov), the Los Alamos National Laboratory, the Lawrence Livermore National Laboratory, and the National Center for Scientific Research "Demokritos" in Greece, has brought the students into contact with Ph.D.-granting institutions and national laboratories, and has enhanced the research environment at CSUN.

V. Computational Materials Center Facilities

A theoretical/computational materials research center was recently established at CSUN comprised of professors, postdoctoral fellows, visiting scientists and students. The goals of the center are to conduct high level basic and applied research that enhances our knowledge in condensed matter/materials science; to educate and train students through a program of studies and research activities on materials-related technological challenges of the future; and to stimulate and develop strong industry/university/ national laboratory partnerships in condensed matter/materials research.

The University has allocated 4,000 square feet of space for the Center on the third floor of Science I building. The remodeling of the space was completed Fall 1997. The cost of the remodeling was \$350,000 and was funded by the University. The Center has the following high performance computers:

1. Two Hewlett Packard 735, two Hewlett Packard 712 and ten Hewlett Packard X-terminals. These workstations were purchased from a California State University Northridge grant award (1993) in the amount of \$255,000.
2. Six Hewlett Packard J282 purchased from a W.M. Keck Foundation grant award (1996) in the amount of \$155,000.
3. One Silicon Graphics Octane purchased from internal funds in the amount of \$30,000.
4. A six processor Silicon Graphics Origin 2000 parallel computer purchased from a Ralph Parsons grant award (1998) in the amount of \$95,655.
5. Ten additional processors for the Silicon Graphics Origin 2000 parallel server purchased from a US Army grant award (1999) in the amount of \$199,200.

The latter workstations have some of the highest performance available today and are about only two times slower than the fastest single processor supercomputers such as the Cray C-90. As a result of the growth in both the equipment and the personnel in the Computational Materials Theory Center, as of January 1999, the University has committed a half-time system administrator to maintain the high performance computers.

VI. Bibliography

1. *Chemical Bonding and Elastic Constants of Nickel-Based Intermetallics*, N. Kioussis, J. Blanco, S. P. Lim, and R. Wu, in *Properties of Complex Inorganic Solids*, eds. A. Gonis, A. Meike, and P. Turchi, 389 (Plenum, New York, 1997).

2. *First principles determination of hyperfine fields in Pt/Fe (111) multilayers.* G. Lu, R. Wu, L. Chen, and N. Kioussis. *NATO ASI Magnetic Hysteresis in Novel Magnetic Materials, Series E.* **338**, 179 (1997).
3. *Ab initio electronic structure of the $\Sigma 5$ Grain Boundary in Ni₃Al.* G. Lu and N. Kioussis, *Mater. Res. Soc. Symp. Proc.* **472**, (1997).
4. *First principles investigations of 4d magnetism on C(0001).* L. J. Chen, R. Wu, N. Kioussis, and J. Blanco, *J. Appl. Phys.* **81**, 4161 (1997).
5. *Electronic mechanism of oxygen embrittlement of TiAl,* Y. Liu, K.Y. Chen, J. H. Zhang, Z. Q. Hu, G. Lu, and N. Kioussis. *J. Phys. Cond. Matter. Phys.* **9**, 9829 (1997).
6. *One-dimensional Hubbard Model in the presence of magnetic field.* N. Kioussis, A. Kocharian, and S. Park. *J. Magn. Magn. Mater.* **177-181**, 575 (1997).
7. *First principles determination of the bonding mechanism and adsorption energy for CO/MgO (001).* L. Chen, R. Wu, N. Kioussis, and Q. Zhang, *Chem. Phys. Lett.* **290**, (1998).
8. *First principles studies of the $\Sigma 5$ tilt grain boundary in Ni₃Al,* G. Lu, N. Kioussis, R. Wu, and M. Ciftan, *Phys. Rev. B* **59**, 891 (1999).
9. *Ab initio study of anisotropic magnetism in Uranium compounds,* E. Collins, N. Kioussis, and S. P. Lim. *J. Appl. Phys.* **85**, 6226 (1999).
10. *Effect of hydrogen on grain-boundary embrittlement: An ab initio study.* G. Lu, N. Kioussis, R. Wu, and M. Ciftan, in *Condensed Matter Theories*, **15**, (Nova, Spring 2000, in press).
11. *Tight-binding study of stacking faults and the Rice criterion of ductility in the fcc metals,* M. Mehl, D. Papaconstantopoulos, N. Kioussis, and M. Herbranson. *Phys. Rev. B* **61**, 4894 (2000).
12. *Generalized stacking fault energy surfaces and dislocation properties of Aluminum,* G. Lu, N. Kioussis, V. Bulatov, and E. Kaxiras. *Phys. Rev. B* **62**, 3099 (2000).
13. *Monte Carlo simulations of grain boundary sliding: Effect of vacancies,* P. Ballo, N. Kioussis, and G. Lu, to be submitted to *J. Mater. Research* (2000); *Effect of a vacancy on grain boundary sliding,* G. Lu and N. Kioussis, submitted to *Phys. Rev. B* (2000).
14. *Development of Magnetism in Strongly Correlated Electron Systems: Non-Kondo mechanism for moment collapse.* E. Collins, N. Kioussis, S. P. Lim, and B. R. Cooper. *Phys. Rev. B* **62**, 11533 (2000).
15. *Interplay between crystal field and exchange interactions in strongly correlated Cerium systems,* E. Collins, N. Kioussis, S. P. Lim, and B. R. Cooper, *J. Appl. Phys.* **87**, 5143 (2000).
16. *The Peierls-Nabarro model revisited,* G. Lu, N. Kioussis, V. Bulatov, and E. Kaxiras, *Phil. Mag. Lett.* **80**, 675 (2000).
17. *Correlation of topology of charge density and stability of planar faults in metals,* N. Kioussis, M. Herbranson, and M. Eberhart, to be submitted to *Phys. Rev. B* (2000).

18. *High Temperature Ordered Intermetallic Alloys*, edited by N. S. Stoloff, C. C. Koch, C. T. Liu and O. Izumi. MRS Symposium Proceedings, Vol. 81. (Materials Research Society, Pittsburgh, 1987).
19. C. T. Liu and D. P. Pope in *Intermetallic Compounds - Principles and Practices*, ed. by J. H. Westbrook and R. L. Fleischer. (Wiley, New York, 1995), Vol. 2, p.17.
20. T. Takasugi and O. Izumi. Acta Metall. 31, 1187 (1983); Takayuki Takasugi, in *Intermetallic Compounds - Principles and Practices*, edited by J. H. Westbrook and R.L. Fleischer. (John Wiley & Sons, 1995), Vol. 1, p 585.
21. K. Aoki and O. Izumi, J. Jpn. Inst. Met. **43**, 1190(1979).
22. C. T. Liu, C. L. White and J. A. Horton. Acta Metall. **33**, 213 (1985).
23. E. P. George, C. T. Liu and D. P. Pope, Scripta Metall. Mater. **27**, 365 (1992).
24. J. R. Rice and J. S. Wang. Mater. Sci. Eng. A **107**, 23 (1989).
25. M. S. Duesbery and G. Y. Richardson, Solid State and Materials Sciences, **17**, 1 (1991).
26. V. Vitek, Progress in Materials Science, **36**, 1 (1992).
27. B. Joacutcos, Q. Ren, and M. S. Duesbery. Phys. Rev. B **50**, 5890 (1994).
28. Y. Juan and E. Kaxiras. Phil. Mag. A **74**, 1367(1996).
29. V. V. Bulatov and E. Kaxiras. Phys. Rev. Lett. **78**, 4221 (1997).
30. J. R. Rice and R. Thomson. Philos. Mag. **29**, 78 (1974).
31. M. E. Eberhart. Phil. Mag. A **73**, 47 (1996); M. E. Eberhart and A. F. Giamei. Mater. Scien. and Eng. **A248**, 287 (1998).
32. Siu-Wai Chan and V.S.Boyko. Phys.Rev. B **53**, 16, 576 (1996).
33. A. P. Sutton and E. W. Balluffi, *Interfaces in crystalline materials*, p. 475 (Oxford University Press, 1995).
34. D.Wolf, J.Appl.Phys. **68**, 3221 (1990).
35. J. Wadsworth, O. A. Ruano, and O. D. Sherby, preprint. UCRL-JC-132348 (1999).
36. J. Rossat-Mignod, P. Buriel, S. Quezel, J. M. Effantin, D. Delacote, H. Bartholin, O. Vogt, and D. Ravot, J. Magn. Magn. Mater. **31-34**, 398 (1983).
37. J. Rossat-Mignod, J. M. Effantin, P. Buriel, T. Chattopadhyay, L. P. Regnault, H. Bartholin, C. Vettier, O. Vogt, D. Ravot, and J. C.Achart. J. Magn. Magn. Mater. **52**, 111 (1985).
38. H.R. Krishnamurthy, C. Jayaprakashh, S. Sarker, W. Wenzel. Phys. Rev. Lett. **64**, 950 (1990).
39. R. Strack, D. Vollhardt. Phys. Rev. B **72**, 3425 (1994).

40. J.R. Schrieffer, X.-G.Wen, and S.-C.Zhang, Phys. Rev. Lett. **60**, 944 (1988).
41. E. Lieb, and F. Wu, Phys. Rev. Lett. **20**, 1445 (1968); M. Takahashi, Progr. Theor. Phys. **43**, 1619 (1970).