

**Chapter 1 : Atomic-scale engineering of the SiC-SiO<sub>2</sub> interface © SOFI Northwestern**

*A wide variety of properties of materials are determined by processes which take place on an atomic scale. In recent years, theoretical developments and advances in computer power have made it.*

Taylor, almost simultaneously realized that plastic deformation could be explained in terms of the theory of dislocations. Dislocations can move if the atoms from one of the surrounding planes break their bonds and rebond with the atoms at the terminating edge. In effect, a half plane of atoms is moved in response to shear stress by breaking and reforming a line of bonds, one or a few at a time. The energy required to break a single bond is far less than that required to break all the bonds on an entire plane of atoms at once. Even this simple model of the force required to move a dislocation shows that plasticity is possible at much lower stresses than in a perfect crystal. In many materials, particularly ductile materials, dislocations are the "carrier" of plastic deformation, and the energy required to move them is less than the energy required to fracture the material. Dislocations give rise to the characteristic malleability of metals. The consequent increasing overlap between the strain fields of adjacent dislocations gradually increases the resistance to further dislocation motion. This causes a hardening of the metal as deformation progresses. In addition, adding pinning points that inhibit the motion of dislocations, such as alloying elements, can introduce stress fields that ultimately strengthen the material by requiring a higher applied stress to overcome the pinning stress and continue dislocation motion. The effects of strain hardening by accumulation of dislocations and the grain structure formed at high strain can be removed by appropriate heat treatment annealing which promotes the recovery and subsequent recrystallisation of the material. The combined processing techniques of work hardening and annealing allow for control over dislocation density, the degree of dislocation entanglement, and ultimately the yield strength of the material.

**Climb** [ edit ] Dislocations can slip in planes containing both the dislocation line and the Burgers vector. For a screw dislocation, the dislocation line and the Burgers vector are parallel, so the dislocation may slip in any plane containing the dislocation. For an edge dislocation, the dislocation and the Burgers vector are perpendicular, so there is one plane in which the dislocation can slip. There is an alternative mechanism of dislocation motion, fundamentally different from slip, that allows an edge dislocation to move out of its slip plane, known as dislocation climb. Dislocation climb allows an edge dislocation to move perpendicular to its slip plane. A creep mechanism involving only dislocation climb, also known as Harper-Dorn creep, can occur under certain conditions. If a vacancy moves next to the boundary of the extra half plane of atoms that forms an edge dislocation, the atom in the half plane closest to the vacancy can "jump" and fill the vacancy. This atom shift "moves" the vacancy in line with the half plane of atoms, causing a shift, or positive climb, of the dislocation. The process of a vacancy being absorbed at the boundary of a half plane of atoms, rather than created, is known as negative climb. Since dislocation climb results from individual atoms "jumping" into vacancies, climb occurs in single atom diameter increments. During positive climb, the crystal shrinks in the direction perpendicular to the extra half plane of atoms because atoms are being removed from the half plane. Since negative climb involves an addition of atoms to the half plane, the crystal grows in the direction perpendicular to the half plane. Therefore, compressive stress in the direction perpendicular to the half plane promotes positive climb, while tensile stress promotes negative climb. This is one main difference between slip and climb, since slip is caused by only shear stress. One additional difference between dislocation slip and climb is the temperature dependence. Climb occurs much more rapidly at high temperatures than low temperatures due to an increase in vacancy motion. Slip, on the other hand, has only a small dependence on temperature.

## Chapter 2 : Dislocation - Wikipedia

*Introduction: the role of computations in materials science* With the rapid development of advanced technologies in all areas, from light-weight constructions in the automotive and aircraft industries over very large-scale integration in microelectronics (and the upcoming nanoelectronics) to the chemical and biomedical industries, advanced materials science is confronted with the need for an.

Thus, a fundamental goal of theoretical work in materials science is the description of properties of bulk materials based only on the properties of and interactions between their constituent atoms and molecules. During the last 40 years, tremendous progress has been made toward this goal of understanding and predicting material properties from such a microscopic viewpoint. Research of this nature falls into several broad categories as follows: Crystalline materials are characterized by having all the constituent atoms arranged about fixed positions in a periodic lattice. Thus, given the known atomic arrangements, as obtained, say, from x-ray diffraction experiments, theory seeks both to predict and to explain experimental observations concerning the electronic, optical, magnetic, transport, and other properties of these crystalline materials. While a number of other materials have their constituent atoms and molecules arranged about fixed positions, these positions are not known in advance and are the desired objects of theory. Such systems involve surfaces of materials, where the surface atoms often rearrange themselves from the bulk configurations, defects in materials such as dopants in semiconductors, where the host atoms generally alter their arrangement in response to the guest, and folded proteins, where the molecule is found in a complicated equilibrium globular structure that is related to its biological activity. Theories of these materials must first be capable of determining the equilibrium arrangements of atoms before researchers can study a host of other properties of these materials. Liquids and glasses, on the other hand, have more complicated arrangements of the constituent atoms and molecules. Liquids owe their fluidity to the fact that the constituent atoms are not centered about fixed positions but are slowly able to diffuse through the whole system. Thus, theories of liquids seek to determine the statistical properties of the equilibrium atomic and molecular configurations. Many systems are not in thermal equilibrium, and the object of theory becomes a desire to calculate the dynamical evolution of a nonequilibrium assembly of atoms and molecules. The ultimate theory in all three cases would proceed completely from first principles, using quantum mechanics to describe electrons, spins, and nuclear motions. This has been the object of solid-state physics theories for crystalline materials, where the nuclei undergo only small-amplitude vibrations about equilibrium positions. However, when the nuclei are permitted to move over more substantial distances, such as in the examples described in 2 above, it is often adequate to treat the nuclear motion in terms of classical equations of motion, with the forces between atoms and molecules calculated using quantum mechanics or, when unavailable, from empirical potential functions. The latter is the realm of conventional molecular dynamics Abraham, , which has been applied to a wide variety of systems, including surface reconstruction, liquid and glass structures and dynamics, and others. In many other systems, the interatomic forces depend too intimately on nuclear Page 6 Share Cite Suggested Citation: Mathematical Research in Materials Science: The National Academies Press. Cohesive energies, of solids, for instance, are obtained from differences in eigenvalues of this equation for the solid and the separated atoms, but the accuracy of solution required is enormous because this cohesive energy represents only on the order of of the total eigenvalue. Density functional theory Hohenberg and Kohn, ; Kohn and Sham, ; Callaway and March, ; see also Interfaces in Polymer Systems in Chapter 3 provides a framework for the calculation of the electronic structure and total energy of any solid-state or molecular system. However, the underlying Hohenberg-Kohn theorem only proves the existence of the density functional, but does not describe its exact form. Thus, various approximate and heuristic density functionals are used in practice. Rather little has been done to compute these density functionals from first principles theory Levy, ; Freed and Levy, , and mathematical assistance would be welcomed see Chapters 3 and 8 in proving theorems concerning

properties of density functionals Levy, and in developing new approximation schemes as means for systematically improving available and perform approximate density functional methods. The problem is usually solved iteratively until self-consistency is achieved between the eigenfunctions and the potential energy. The development of fast Fourier transform methods has been a key mathematical contribution to improving the efficiency of this process. The eigenfunctions and eigenvalues are then used to calculate densities of states, optical spectra, carrier life times, and so forth. Most implementations of density functional methods employ what is called the local-density approximation to incorporate exchange and correlation in the effective single-particle potential energy. In recent years, a number of methods, including quantum Monte Carlo approaches Zhu and Louie, , have been developed to go beyond this approximation, resulting in significant improvement in the calculated electron energy levels. The main theoretical problem here lies in extrapolating solutions for small clusters to the bulk or in extracting parameters for model Hamiltonian treatments of, for instance, high-temperature superconductivity. Page 7 Share Cite Suggested Citation: A calculation of the total energy as a function of small deviations from perfect crystallinity enables the computation of the vibrational spectra phonons of the solid. When the lowest-energy atomic arrangement is unknown in advance and is to be calculated, computation of the electronic energy for this configuration of the atoms enables determination of the total forces on each atom in the system. These forces are then used to calculate the configuration of minimum energy either by employing energy-minimization techniques or by seeking a configuration in which forces on all atoms vanish. Earlier approaches involved the repeated solution of the self-consistent electronic eigenvalue problem for each atomic arrangement encountered in the energy minimization process. Recently, a number of techniques have been developed in which the electronic and nuclear degrees of freedom are treated simultaneously Car and Parrinello, ; Payne et al. These techniques have resulted in vast improvements in efficiency for the computation of both equilibrium configurations and dynamics. Other advances enable the treatment of complex materials Ellis et al. For perfect periodic crystals, the size of the problem is determined by the number of atoms in the primitive unit cell. When periodicity is broken by the presence of surfaces, interfaces, and defects, the problem becomes mathematically more complex. A number of methods have been developed to handle this reduced symmetry. With the advent of very powerful computers, however, these techniques have lost ground to a simpler approach based on supercells. For example, a large cell containing a point defect is repeated periodically. The cells must be large enough so that interactions between defects in neighboring cells are insignificant. Similarly, studies of surface properties or of interfaces use periodically repeated slabs. Solutions are typically constructed by expanding the eigenfunctions in terms of a basis set. A variety of basis sets have proven useful in different cases, but the power of modern computers favors the use of plane waves because the size of the basis set can be increased systematically until convergence is achieved Ihm et al. The treatment of dynamical properties, such as conductivity, is generally carried out with semiempirical Hamiltonians, for example, a tight-binding Hamiltonian that is constructed with a localized basis set of atomic orbitals Khan and Broughton, The Hamiltonian is defined in terms of its matrix elements, but there are major conceptual and mathematical problems associated with the theoretical determination of these Hamiltonian matrix elements; these offer research opportunities. When material properties may adequately be computed by first averaging out the electrons, the difficult task still remains of constructing suitable interatomic potentials Baskes et al. Analytical expressions are typically assumed that incorporate pairwise interactions plus additional many-body terms, depending on the nature of the material. The parameters in the potentials are tuned to reproduce either experimental data for example, lattice constants, elastic constants, and so on or theoretical results calculated by first-principles techniques. Once constructed, the interatomic potentials are used to predict a variety of other equilibrium and dynamical properties of both the Page 8 Share Cite Suggested Citation: Similar approaches are applied to the description of polymers, proteins, and glasses. The construction of accurate and reliable interatomic potentials remains a pressing problem that can benefit from new mathematical sciences research. First-principles calculations provide an enormous database concerning the interaction potentials.

However, the construction of computationally convenient interatomic potentials involves a many-parameter, highly nontrivial, nonlinear fitting problem. Currently, the frontiers in atomic-scale theories concern the computation of equilibrium atomic configurations and the evolution of nonequilibrium configurations at nonzero temperatures. The former is usually carried out with direct energy minimization techniques or with Monte Carlo simulation methods. The latter is carried out using molecular dynamics, which can be implemented with a first-principles Hamiltonian, a semiempirical tight-binding Hamiltonian, or with interatomic potentials. The method is in effect an implementation of statistical mechanics. In order to calculate the evolution of a system, externally controlled variables such as pressure or volume, temperature, and so on must be specified. Such specification defines a statistical mechanical ensemble, and the calculation simulates the evolution of a single member of the ensemble in terms of the "trajectories" of all the particle coordinates and momenta in phase space. Equilibrium properties are calculated as time integrals. In addition, elastic constants and linear transport coefficients are obtained using formulas derived from fluctuation theory. Finally, the detailed dynamical evolution allows one to unravel the atomistic mechanisms that underlie a variety of processes and phenomena. For example, studies have been made of dislocation formation and motion, plastic flow, grain boundary sliding and strengthening, crack propagation, tribological phenomena, chemical reactivity, and so forth. Landman et al. The mathematical sciences have made valuable contributions to the developments described above, especially to the numerical implementations. Examples are fast Fourier transforms, multidimensional integration, curved-space description Riemannian metric, solutions of nonlinear equations, nonlinear regression, conjugate-gradient methods, and eigenvalue methods for large or sparse matrices. The main limiting factors in computational atomic-scale research today are the number of atoms that can be treated and the length of the simulation. Parallel computers are becoming an important ingredient in the impetus to study larger systems. The current limits are a few hundred atoms for first-principles calculations and several hundred million atoms for conventional molecular dynamics using interatomic potentials. In time scales, first-principles calculations are limited to picoseconds, whereas conventional molecular dynamics is limited to nanoseconds. Mathematical challenges lie in the development of algorithms to handle large numbers of atoms, in the analysis of instabilities that may arise in the governing equations, and in the development of general asymptotic methods to pass to larger scales. The above does not exhaust interesting areas involving electronic structure and other atomic-scale theories for properties of materials. One other area is electron transport. In most cases, the classical Boltzmann transport equation is adequate, with the electrons and Page 9 Share Cite Suggested Citation: The drift-diffusion approximation has been the workhorse of the microelectronics industry in modeling devices Cole et al. At the next level of sophistication, the hydrodynamic approximation, more accurate solutions are possible Blotekjaer, ; Rudan and Odeh, Finally, exact solutions of the Boltzmann equation are possible by Monte Carlo techniques Jacoboni and Reggiani, ; Fischetti and Laux, , Mathematicians played key roles in many of these developments. Computer implementations of the Monte Carlo techniques are, however, extremely time consuming, calling for the development of more efficient algorithms see Chapter 8. Some currently available mathematical results may provide new inspiration to materials scientists if this well-known mathematics is brought to their attention. A recent example is the study of graphite-like carbon structure with negative Gaussian curvature Mackay and Terrones, Construction of such structures depends on the mathematics of periodic minimal surfaces that was developed more than a century ago Schwarz, ; Weierstrass, These minimal surfaces are also relevant to the study of microphase separation in block copolymer systems see Chapter 3. Strong electronic correlations play a dominant role in phenomena such as the metal-nonmetal transition and probably high-temperature superconductivity. Standard density functional theory in the local density approximation does not accommodate these strong correlations, and even ab initio quantum mechanical methods encounter difficulties when many electrons must be correlated. Typically, one has to construct a model theory that captures the essence of the strong correlations. Quite often, a model theory, though simple in appearance, may present significant mathematical challenges to obtaining practical solutions to specific problems. Performing direct numerical calculations for the many-body

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problem of strongly correlated electrons is another frontier. The main limitation is again on the number of electrons that can be accommodated. There are efforts to construct model Hamiltonians with reduced degrees of freedom by introducing a mapping from the true Hamiltonian McMahan et al. Some progress, however, is available for small-molecule systems Freed, , Further mathematically rigorous developments in this area would be very valuable. Many workers have explored methods beyond density functional methods in order to describe quantum effects for systems in which material properties involve excited states, be they optical or high thermal excitations. Wiener path integral methods have been extensively used to model Chandler and Wolynes, ; Berne and Thirumalai, the thermal properties of the solvated electron Rossky and Schnitker, , the role of quantized rotational and librational motion in liquid water Kuharski and Rossky, , superfluid transitions in liquid helium Ceperley and Pollock, , melting in rare-gas clusters Doll et al. Simulated annealing techniques have enabled the computation of electronically excited potential surfaces in conjunction with molecular dynamics simulations of the nuclear motion. Simulated annealing has been applied to the Na<sub>4</sub> cluster using a generalized valence bond electronic wavefunction, but only a femtosecond test run has been reported so far Hartke and Carter,

## Chapter 3 : Materials Science Suite | Schrödinger

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## Chapter 4 : Atomic-scale materials design - DTU Physics

*Atomic Scale Calculations in Materials Science: Symposium Held November 28 - December 1, , Boston, Massachusetts, U.S.A. (Materials Research Society Symposium Proceedings) Hardcover - May 1,*

## Chapter 5 : Project to elucidate the structure of atomic nuclei at the femtoscale

*Atomic-scale theories have proved to be very valuable in elucidating the properties of all sorts of materials. Electronic structure calculations have been essential in understanding electronic, optical, and transport properties, including elastic constants, conductivities, magnetic properties, and many more.*