microscopy. Thermodynamic arguments for the existence of the superlattice phases will be presented. We will relate the experimental data to appropriate models and indicate problems which deserve more fundamental attention.

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CP 5

Bistability and Multistability

Bistability, e.g., as in current-voltage characteristics, occurs in many of the new semiconductor devices, photorefractive materials, ferroelectric liquid crystals, polyesters, surface stabilized light valves, FLC SLM VLSI miniaturizations, and elsewhere in the new material sciences. It may be desirable or undesirable depending on the situation. Closer analysis can reveal midrange multistabilities, which also may or may not be of good use. I will present an example, and discuss the issues it brings out.

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Stability of Cylindrical Bodies in the Theory of Surface Diffusion

It is shown that the classical result in the linearized theory of the stability of cylinders against surface diffusion, to the effect that an unperturbed cylinder is stable against all sinusoidal perturbations of wavelength less than the circumference, must be modified when nonlinear effects are taken into account. Numerical solutions of the full nonlinear equations are presented and compared with the results of a perturbation analysis.

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Modelling and Simulation of Reaction and Diffusion in a Corrosion Cell

Ionic transport processes in bulk chloride solutions have been successfully modelled by coupled time-dependent reaction-diffusion equations with the dependent variables being the concentrations of various constituent molecular or ionic species and the electrostatic potential. The model system comprises an iron surface in contact with an enclosed acetic acid volume. The coupled partial differential equations are solved via semi-implicit methods. Species enter the model system as time-dependent boundary conditions on the sample.

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Nonlinear Diffusion from a Lattice-Gas Model

The molecular basis for nonlinear diffusion coefficients is investigated. A lattice-gas model, subject to exclusion of double occupancy, is used to obtain a set of differential equations for the single-site occupancies. Coverage-dependence of the diffusion coefficient are determined. This approch is extendable to situations in which kinetics are important.

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An Advanced Model for Dopant Diffusion in Polysilicon

Polysilicon thin films are widely used in integrated circuit fabrication processes as diffusion sources, which leads to a demand on an accurate numerical diffusion model. We take into account dopant diffusion in grains, in grain boundaries as well as in the single crystal silicon substrate. Due to the complex grain structure of polysilicon, dynamic dopant segregation between the grain and the grain boundary has to be included. Dynamic grain growth and a trapping/emission mechanism are the dominating effects. To model these requirements the conventional nonlinear diffusion PDEs are coupled with a partial differential equation for grain growth and an algebraic equation to calculate the active dopant concentration. The polysilicon grains itselfs are assumed to be tiny squares, growing from initial size. In order to handle nonplanar semiconductor structures, we use a transformation method for the simulation area as well as for the PDEs.

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CP 6

Wave Propagation in Some Chiral Composite Materials

We consider the scattering for an electromagnetic wave by a chiral material. The behavior of electromagnetic waves in a composite material wich is componed as a mixture of two chiral materials is also investgated. In such a case, the model leads to a problem of homogenization in periodical structure. Zero and first order terms are computed and error estimates are given using a variational method. Validity of constitutive laws is discussed.

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Wave Propagation Along Grain Boundaries

Interfacial wave propagation is investigated in terms of phonons (for discrete bicrystal superlattices) and wave solutions (for continuum analog). Perfect bonding solutions are too restrictive since only specific velocities for limited propagation directions are possible. In contrast, solutions for spring and membrane interfacial models with certain admissible displacement and traction jumps are dispersive and exist for any propagation direction. As an example, gold and copper anisotropic bicrystals are studied using Stroh's complex variable formalism. The differences in localization of acoustical phonons for gold (localized) and copper (not localized) are explained by difference in interface properties derived from atomistic calculations of grain boundary properties.

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