JOURNAL OF COMPUTATIONAL PHYSICS 112, 210 (1994)

Abstracts of Papers to Appear in Future Issues

USE OF PARTIAL KNOWLEDGE OF THE POTENTIAL IN THE PHASE PROBLEM OF INVERSE SCATTERING. Michael V. Klibanov. *University of North Carolina at Charlotte, Charlotte, North Carolina 28223, U.S.A.*; Paul E. Sacks. *Iowa State University, Ames, Iowa 50011, U.S.A.*

We consider the problem of determining a potential $V(x)$ in the one-dimensional Schrödinger equation, given as data the reflectivity $r(k) = |R(k)|^2$, where $R(k)$ denotes the usual quantum mechanical reflection coefficient. It is well known that in the absence of phase information, there can be a considerable degree of nonuniqueness, which is closely connected to the presence of zeros of $R(k)$ in the upper half of the complex plane. Some earlier work of the authors showed that this ambiguity can be resolved by providing a small amount of extra information about the potential. In this article we develop a computational technique, based on an optimization approach to the problem of locating the zeros of $R(k)$. Some numerical examples are given.

MOLECULAR DYNAMICS SIMULATIONS OF THE EFFECTS OF DAMAGE RELAXATION FOLLOWING HIGH-ENERGY IMPLANTS. A. M. Mazzone. *C.N.R., Istituto Lamel, Via de' Castagnoli, Bologna, I-40126, Italy.*

This work presents a molecular dynamics simulation method designed to describe the processes of electron and lattice relaxation taking place in the typical cascade volumes formed by high-energy implants. The simulation method is based on classical mechanics and includes the motion of electrons and nuclei. The results are in agreement with experimental observations.

A TRULY NONINTERPOLATING SEMI-LAGRANGIAN LAX–WENDROFF METHOD. M. Olim. *Institute of Fluid Science, Tohoku University, Sendai, Japan.*

A truly noninterpolating semi-Lagrangian method has been developed. It is based upon a modification of a standard Lax–Wendroff scheme and is unconditionally stable on a regular rectangular grid. The method is explicit and second-order accurate in both time and space. It is suggested that the computational cost and memory allocation required by this method are the least possible for a semi-Lagrangian algorithm of this order of accuracy. The numerical experiments presented indicate that the algorithm is very accurate indeed.

COMPUTER SIMULATION OF COIL DEFORMATION. S. Kreitmeier, M. Wittkop, and D. Göritz. *Universität Regensburg, Institut für Angewandte Physik, Universitätsstr. 31, D-8400 Regensburg, Germany.*

The deformation behavior of statistical coils in the condensed state were studied by computer simulations. The simulated systems consisted of single and double chains, each with $(N-1)$ segments, which could rotate about their junctions. Van der Waals interactions were considered between all junctions. Equilibrium conformations were obtained by potential energy minimization using a modified Newton algorithm. During the simulated deformation, all initial coils transformed into a highly oriented fibril and a residual coil. Combining the behaviour of several coils, the energy increased nearly linearly with the extension ratio and due to this the retractive force was independent of the extension rate.

NOTE TO APPEAR

REMOVING SMALL FEATURES FROM COMPUTATIONAL DOMAINS. Joseph B. Keller. *Stanford University, Stanford, California 94305, U.S.A.*

Printed in Belgium
Uitgever: Academic Press, Inc.
Verantwoordelijke uitgever voor België:
Hubert Van Maele
Altenastraat 20, B-8310 Sint-Kruis

0021-9991/94 $6.00