PACKAGE ID - 000788MLTPL00 DYNAMO

KWIC TITLE - Molecular Dynamics and Energy Minimization Based on Embedded Atom Method

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LIMITATION CODE -UNL **AUDIENCE CODE -** UNL

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DESCRIPTION - This program performs atomic scale computer simulations of the structure and dynamics of metallic system using energetices based on the Embedded Atom Method. The program performs two types of calculations. First, it performs local energy minimization of all atomic positions to determine ground state and saddle point energies and structures. Second, it performs molecular dynamics simulations to determine thermodynamics or miscroscopic dynamics of the system. In both cases, various constraints can be applied to the system. The volume of the system can be varied automatically to achieve any desired external pressure. The temperature in molecular dynamics simulations can be controlled by a variety of methods. Further, the temperature control can be applied either to the entire system or just a subset of the atoms that would act as a thermal source/sink. The motion of one or more of the atoms can be constrained to either simulate the effects of bulk boundary conditions or to facilitate the determination of saddle point configurations. The simulations are performed with periodic boundary conditions.

PACKAGE CONTENTS - Media Directory; Software Abstract; Media Includes Source Code, User's Guide, Executable Module, Auxiliary Material, Sample Problem Input and Output;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 Cassette

METHOD OF SOLUTION - The energetics upon which the simulations are based are computed using the Embedded Atom Method as described in detail in the references in Section 15. The energy minimization is performed by standard conjugate gradient techniques with the energy gradients calculated analytically. The molecular dynamics using a standard finite difference algorithm to advance the time steps. The simulation at constant pressure is accomplished using the algorithm of Parinello and Raham. The fixed temperature simulations are performed either by imposing a fictitious drag term that depends on the deviation of the current temperature from the desired temperature or by the Langevin method of imposing random impulsive

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METHOD OF SOLUTION -(CONT) forces on the atoms.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - Version provided was compiled and tested using SunOS 4.1.3 and the SunPro F77 compiler version 2.0.1. No modifications of the OS or compiler were made.

PROGRAMMING LANGUAGES - FORTRAN 77 with Namelist input extensions.

SOFTWARE LIMITATIONS - The number of atoms that can resonably be simulated is limited to about 50,000.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - The code provides a much more convenient user interface compared to similar codes. Unlike many competing packages, the imposition of constraints and temperature control does not require the modification of the source code. The code incorporates the ability to generate simple crystalline lattices and a simple method for incorporating defects such as additional atoms, vacancies, atomic displacements, etc. The code provides multiple methods for imposing temperature constraints and is unusual in the features of being able to impose those constraints on a subset of atoms.

RELATED SOFTWARE - In some applications, software may be required to generate complex initial atomic positions. The program CREATOR written by Murray S. Daw would serve that need. The empirical functions used by the Embedded Atom Method for the late transition metals are included in tabular form in this distribution. There is not a general purpose program for generating these functions for other materials and/or based on other data.

OTHER PROG/OPER SYS INFO - No additional software libraries are required.

HARDWARE REQS - Hardware requirements depend strongly on the details of the simulation to be performed. The RAM required vaires from about 10 Mbytes for system sizes of 2000 atoms to about 120 Mbytes for systems of 50000 atoms. The disk memory requirements small(<10 Mbytes) unless one wants to store the atomic trajectories for long molecular dynamic simulations.

TIME REQUIREMENTS - A single evaluation of the energy and forces requires about 0.5 CPU seconds on a Sun Sparc 10/51 workstation for a system of about 1000 atoms. The cpu time requires scale aproximately linearly with the number of atoms. An energy minimization typically requires ten to hundreds of energy/force evaluations. A molecular dynamics requires one such evaluation for each time step. Typical time steps for metallic systems are about 5

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TIME REQUIREMENTS -(CONT) femtoseconds of simulated time.

REFERENCES - User's Guide on media

SUBJECT CLASS CODE - Q

KEYWORDS -
COMPUTER PROGRAM DOCUMENTATION
D CODES
CRYSTAL STRUCTURE
DISPLACEMENT RATES

EDB SUBJECT CATEGORIES -
990200 665000 360102

SPONSOR - DOE/ER

PACKAGE TYPE - SCREENED