

Kalypso: a software package for molecular dynamics simulation of atomic collisions at surfaces

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Abstract

A suite of graphically-oriented computer programs (Kalypso) has been developed for molecular dynamics simulations of projectile collisions with metallic targets. The features of the package include free-boundary or periodic targets, many-body potentials, a variety of inelastic loss models, and the ability to carry out simulations of fluence-dependent processes.

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1. Introduction

Laboratory and industrial techniques that exploit ion bombardment phenomena rely on numerical models for interpretative and/or predictive purposes. Bombardment phenomena of practical interest span a wide range of length and time scales that no single modelling approach can cover. Molecular dynamics (MD) is well-suited for modelling bombardment phenomena that involve short time and length scales ($<10^{-8}$ s, $<10^{-7}$ m).

This paper describes a software package (Kalypso) for MD simulation of projectile collisions with metallic targets. The package addresses a perceived need for access to MD simulations on a production basis by the experimental ion beam community. Most publicly available MD codes that are suitable for ion beam applications require a substantial level of computing expertise for their successful application. Kalypso comprises an integrated, user-friendly, suite of tools for the design, execution and analysis of ad hoc simulation projects that relate to ion bombardment or atomic recoil processes. The features of the package include many-body potentials, a variety of inelastic loss models, and the ability to carry out simulations

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of fluence-dependent processes. The Kalypso package (version 2), consisting of 32-bit Windows binaries and documentation, may be obtained through the World Wide Web [1].

2. Computer implementation

User interactions with the Kalypso modules take place via a graphical user interface. Visualisation tools are provided to support various aspects of the simulation project, from input data entry to output data analysis. Other tools automate common tasks such as the computation of lattice energies, scattering properties, and surface relaxations. The input data required for a simulation are (a) the initial positions and velocities of target and projectile atoms (including thermal effects), (b) parameters that describe the interatomic potentials and non-elastic processes (see below) and (c) parameters and conditions that control the manner in which the simulation runs and terminates. Kalypso distributes these data among several input files.

The simulation target may consist of 1 or 2 metal atom types. The projectile species is a single noble gas or metallic atom, or a metallic cluster (e.g. Cu_3). Noble gas atoms interact with the target via purely repulsive screened Coulombic potentials. Interactions between metallic atoms are described by means of composite potentials. These potentials consist of a short-range repulsive screened Coulombic potential (V_c) that is interpolated to an attractive, many-body tight-binding (TB) potential [2] (V_a). TB potentials have been fitted for most metals, and for many alloys, but they are not suitable for semiconductor targets (e.g. Si, GaAs). The repulsive and attractive parts of the potential are joined by an interpolation function, $S(r)$:

$$V(r) = V_c(r)S(r) + V_a(r)(1 - S(r)) \quad (1)$$

which is applied in a region $r_1 < r < r_2$, and has the following properties: $S(r_1) = 1$, $S(r_2) = 0$ and $S'(r_1) = S'(r_2) = 0$. All potentials are terminated smoothly at a selected cut-off distance by means of another interpolation function.

Kalypso makes provision for simulation of several energy transfer processes in addition to elastic

scattering. These include discrete (Oen-Robinson, Shapiro-Tombrello) and continuous (Lindhard-Sharff) electronic stopping models, image potential effects, harmonic lattice site springs (e.g. for damping the motion of edge atoms) and temperature control.

After initialisation, the equations of motion of the dynamical system are integrated repeatedly over many time-steps using the Verlet algorithm. Neighbour lists and an adaptive time-step are used to improve the speed of the simulation [3]. Simulations may be carried out on targets with free or periodic boundaries, under conditions of either zero or finite fluence. In the latter mode (multiple impact or MI simulations), the target is not refreshed between projectile impacts, and any implanted projectile species remain embedded in the target. For energetic collision processes, interactions between target atoms may optionally be ignored, with a considerable saving in computation time.

3. Results and discussion

3.1. Benchmarks

Two basic performance characteristics of a simulation program are its accuracy and speed. The program should reproduce established simulation results, and should run at a speed that is useful for practical applications. In this section the performance of Kalypso is benchmarked with respect to two common simulation problems, namely sputtering and impact collision ion scattering spectroscopy (ICISS).

The sputtering of atoms and clusters from Cu(111) by 5 keV Ar projectiles at normal incidence has been examined using a range of MD codes by Colla et al. [4]. This well-documented system has been selected to benchmark the performance and accuracy of Kalypso for sputtering simulations. The Cu(111) target used for this benchmark consisted of 7569 Cu atoms arranged into nine unrelaxed layers, terminated by $\langle 110 \rangle$ free edges, at a temperature of 0 K. An uncorrected ZBL potential described the repulsive Ar–Cu and Cu–Cu interactions. The attractive part

of the Cu–Cu TB potential was cut-off at 4.3 Å. The simulation followed 1107 projectile impacts for 3 ps, and required ~ 10 h of (3.4 GHz) CPU time. Table 1 demonstrates a satisfactory agreement between the sputtered particle yields predicted by Kalypso, and the codes from [4].

ICISS spectra are expensive to simulate because few ($<1\%$) scattering events contribute to the ICISS spectrum. The traditional approach to ICISS simulation has been to use simplified dynamical models for trajectory tracing [5]. Practical ICISS simulations can be carried out with Kalypso using a simplified MD scheme that involves neglect of interactions between target atoms, and the use of periodic boundary conditions. For problems that involve scattering from a single atomic plane (the typical case in ICISS), a simulation rate of $\sim 1.4 \times 10^7$ projectile impacts per hour (3.4 GHz CPU) can be achieved. Fig. 1 compares simulated

and experimental [6] ICISS data for 1.5 keV He⁺ incident on Cu(110) at 130 K along the $\langle 211 \rangle$ azimuthal direction. The simulations employed a relaxed, 6-atom (3-layer) periodic target with Debye–Waller displacements appropriate to 130 K, and a ZBL potential (cut-off at 2 Å) with a screening length correction of 0.75. Simulated data are shown for the two types of $\langle 211 \rangle$ scattering rows that are structurally inequivalent due to relaxation. Each spectrum (4×10^6 impacts) required ~ 15 min of (3.4 GHz) CPU time.

3.2. Multiple impact (MI) simulations

MD simulations have been used extensively to study projectile–surface interactions under conditions of zero fluence. However, the application of MD simulations to fluence-dependent processes is an area of practical interest (e.g. sputter profiling) which to date has hardly been explored. The MI simulation capability of Kalypso permits modelling of the topographic and compositional effects induced by projectile bombardment, which have traditionally been the domain of Monte Carlo codes such as TRIDYN [7].

Fig. 2 illustrates a selection of the information that can be extracted from a MI simulation. The predictions describe the evolution of the composition and topography of the surface of a Cu/Ni(100) target (9.1×10^4 atoms) during sputtering by 2 keV Ar projectiles, and form part of a study of directional effects in sputtering that will be reported in further detail elsewhere. The target consisted of a Ni(100) substrate (34 layers, 2601 atoms per layer) with free boundaries that was covered by a single monolayer (ML) of Cu. The intermetallic TB potentials are described in [2]. Layers 5–33 of the target were maintained at a temperature of 100 K. Atoms in layers 34–35 of the target were anchored at their lattice sites. In the simulation, 221 projectiles impinged sequentially on the target at random points within a circular region of radius 25 Å at 10 ps intervals (each impact corresponds to a fluence of $5.1 \times 10^{12} \text{ cm}^{-2}$).

The topographic and composition data shown in panels A–D of Fig. 2 refer to a region of dimensions $60 \times 60 \text{ Å}^2$ located at the target centre. The

Table 1
Comparison of sputter yields predicted for 5 keV Ar \rightarrow Cu(111) by Kalypso and by other simulation codes [4]

	Kalypso	[4]
Sputter yield, Y	14.1 ± 0.3	13.2–14.1
Dimer yield, Y_2/Y (%)	14.9 ± 0.8	8.9–14.9
Trimer yield, Y_3/Y (%)	2.9 ± 0.4	1.0–3.6

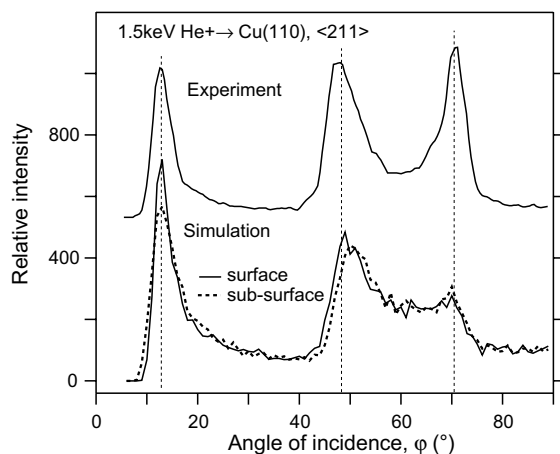


Fig. 1. Simulated and experimental [6] ICISS data for 1.5 keV He⁺ \rightarrow Cu(110) along the $\langle 211 \rangle$ azimuthal direction. The simulated data (178–180° backscattering, $E > 1164$ eV) show contributions from each of the structurally distinct $\langle 211 \rangle$ row types (surface, sub-surface).

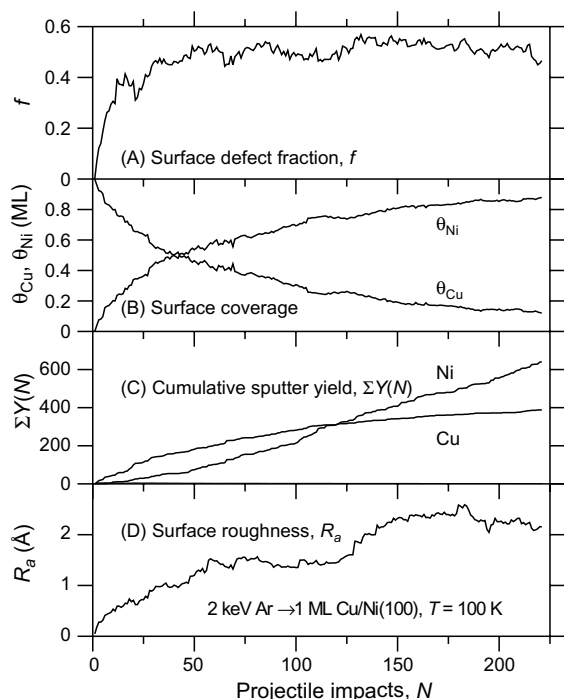


Fig. 2. Sputtering and surface topographic properties predicted by a multiple impact simulation of 2 keV Ar projectiles incident on Cu/Ni(1 0 0) (see text for explanation of terms).

surface defect fraction (panel A) measures the fraction of atoms (crater edge atoms, adatoms etc.) at the surface that have coordination numbers < 8 , i.e. lower than those of ideal surface atoms. The surface coverage (panel B) refers to the composition of atoms in the outermost layer of the target, including any atoms that decorate crater edges. The Cu surface coverage (θ_{Cu}) exhibits initially an exponential decline with projectile fluence until $N = 30$ (corresponding to $\theta_{\text{Cu}} = 0.55$ ML), after which a more gradual decline takes place. The surface defect fraction also attains a steady state value near 0.5 at the same fluence. The cumulative sputter yield curves (panel C) measure the total number of atoms of Cu and Ni removed from the target by sputtering after bombardment by N projectiles (the gradients of these curves represent the sputter yields per projectile). The curves plotted in

panel C intersect at a Cu surface coverage of 0.25 ML after approximately 1.5 ML total erosion of the target. Panel D presents surface roughness predictions that are characterised using the average roughness amplitude, R_a . The latter tends to increase over the entire fluence range investigated, but fluctuates significantly due to a competition between the creation and smoothing of sputter-induced craters.

4. Conclusions

There is growing interest in understanding the dynamical and structural responses of materials to ion bombardment. This requires access to atomistic modelling methods, such as molecular dynamics, that go beyond the binary collision approximation. This paper introduces a simulation package, Kalypso, that can be used for MD simulations of metallic systems under energetic projectile bombardment. The intended audience is the experimental ion beam community. MD simulations of ion bombardment at the zero-fluence limit have been used for many years, but they have never lost their reputation as specialist tools due to the investment of time required to master them. Kalypso has been designed with ease of use in mind. A variety of applications of the package can be envisaged in experimental design, data modelling and predictive engineering.

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