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Dependence of cluster ranges on target cohesive energy: Molecular-dynamics study of energetic Au_{402} cluster impacts

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Abstract

It has long been known that the stopping and ranges of atoms and clusters depends on the projectile-target atom mass ratio. Recently, Carroll et al. [S.J. Carroll, P.D. Nellist, R.E. Palmer, S. Hobday, R. Smith, Phys. Rev. Lett. 84 (2000) 2654] proposed that the stopping of clusters also depends on the cohesive energy of the target. We investigate this dependence using a series of molecular-dynamics simulations, in which we systematically change the target cohesive energy, while keeping all other parameters fixed. We focus on the specific case of Au_{402} cluster impact on van-der-Waals bonded targets. As target, we employ Lennard–Jones materials based on the parameters of Ar, but for which we vary the cohesive energy artificially up to a factor of 20. We show that for small impact energies, $E_0 \lesssim 100$ eV/atom, the range D depends on the target cohesive energy U, $D \propto U^{-\beta}$. The exponent β increases with decreasing projectile energy and assumes values up to $\beta = 0.25$ for $E_0 = 10$ eV/atom. For higher impact energies, the cluster range becomes independent of the target cohesive energy. These results have their origin in the so-called 'clearing-the way' effect of the heavy Au_{402} cluster; this effect is strongly reduced for $E_0 \gtrsim 100$ eV/atom when projectile fragmentation sets in, and the fragments are stopped independently of each other. These results are relevant for studies of cluster stopping and ranges in soft matter.

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1. Introduction

The interaction of clusters with surfaces has received increased attention in recent years. Cluster stopping and the range of clusters in matter are both of a fundamental interest and relevant for applications such as thin-film deposition [1,2], secondary ion and neutral mass spectrometry [3] or as desorption method for biomolecules [4]. Here, also the fate of the cluster and in particular its range are of interest.

Atom ranges have been studied both experimentally and theoretically intensely [5]. They are known to depend on the projectile-target interaction potential, the target atom density and the mass ratio of projectile and target atoms, but not on the target cohesive energy. Less is known about the stopping and range of clusters.

From a theoretical point of view, the stopping of heavy clusters in a light material has been analyzed by Shulga and Sigmund [6]. They found that the range of a heavy cluster is increased beyond that of an equi-velocity atom. The underlying reason is the so-called clearing-the-way effect [7]. The front atoms in the cluster collide with target atoms and convey them sufficient momentum to clear the way for the following cluster atoms. As a consequence the stopping power of the entire cluster is reduced, and hence its range is increased.

Recently, Carroll et al. [8,9] inquired into the stopping of Ag_n clusters ($n = 20$–200) impacting with total energies in the range of 0.5–6 keV into graphite. Their molecular-dynamics results gave evidence that the range D of a cluster

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of energy E_0 per atom and containing n atoms scales as $D \propto E_0 n^{1/3}$. If one assumes [8] that E_0 is mainly spent in breaking bonds of the target solid while penetrating into it, the penetration depth becomes inversely proportional to the cohesive energy U of the target material,

$$D \propto E_0 n^{1/3}/U. \quad (1)$$

The availability of a scaling law such as Eq. (1) would be of immediate interest to the applications mentioned above, since available computer codes like SRIM [10], which work well for monatomic ion ranges, cannot predict cluster ranges.

The applicability of the cluster range formula (1) to a more general cluster stopping scenario has been tested in [11] with a particular emphasis on the cluster size dependence. There, the impact of 100 eV/atom Au_n clusters with n varying in the range of $1 \leqslant n \leqslant 402$ was simulated on a variety of targets, including graphite and a condensed Ar target. It was found that also in this case, ranges follow a power law, $D \propto n^{\alpha}$, where $\alpha = 0.3$–0.4. Quite recently, [12] the nuclear stopping of Au_n clusters was evaluated as a function of cluster size n and impact energy per atom E_0. Since there a larger range of cluster energies was investigated, it could be found that the exponent α – which describes the n-dependence of stopping in analogy to that of the ranges – depends slightly on the impact energy such that with increasing E_0, α goes to zero.

In the present paper, we want to test the dependence of cluster ranges on the target cohesive energy. We focus on a particular system, the impact of Au_{402} clusters on a van-der-Waals bonded target. This situation is representative of irradiation experiments on soft (biological or polymeric) matter.

2. Method

The simulations presented in this paper closely follow our cluster size simulations published previously [11]. The target is modelled as a van-der-Waals-bonded material with a pair interaction potential of the Lennard–Jones form

$$\Phi(r) = 4\epsilon\left[\left(\frac{r}{\sigma}\right)^{12} - \left(\frac{r}{\sigma}\right)^{6}\right], \quad (2)$$

which is cut off at $r_c = 2.5\sigma$. The length parameter is $\sigma = 3.4$ Å. The dimer bond energy ϵ appropriate for Ar is $\epsilon_{Ar} = 10.3$ meV. We note that with our cutoff radius, the cohesive energy of an fcc crystal is $U = 7.9\epsilon = 81$ meV. For $r < 3.4$ Å, we spline the Lennard–Jones potential to the KrC potential [13] valid for close Ar–Ar encounters.

The cohesive energy of our target material is easily changed by choosing different values of ϵ. For our systematic investigations, we chose ϵ/ϵ_{Ar} in the range of 0.5–10, but also performed a few test simulations with increased bonding strength ϵ. Fig. 1 shows the interatomic potentials employed in our study. We note that with increasing ϵ, the spline to the KrC potential is no longer performed so

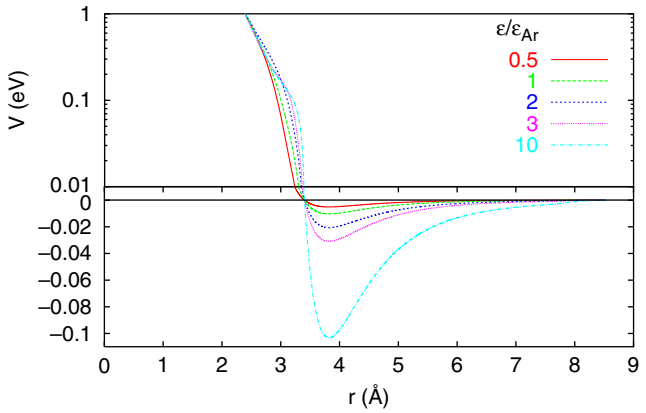

Fig. 1. Interatomic potential $V(r)$ between target atoms as function of interatomic distance r. Note that the ordinate changes from linear to logarithmic scale at positive energies. The parameter ϵ/ϵ_{Ar} characterizes the well depth of the Lennard–Jones potential, Eq. (2), with respect to that of Ar.

easily. Our crystalline fcc target contains 160,000 atoms, has a lateral size of 102×102 Å^2 and a depth of 522 Å; its atomic number density is 0.0295 Å^{-3}.

The 402-atom Au cluster is spherical; the Au–Au interaction potential is of a many-body form [14]. The Au–Ar interaction is purely repulsive according to the ZBL potential [5].

We performed for each impact energy E_0 and for each target a number of five simulations to obtain sufficient statistics. Each simulation uses a different cluster impact point on the target. Since the projectile is quite large, range fluctuations are considerably smaller than for monatomic projectiles, and the accuracy achieved is sufficient for our purpose. We performed simulations both for an amorphous and a crystalline (fcc) target. While the ranges are systematically larger in the amorphous targets, the trends are analogous, and hence we concentrate on the presentation of the crystalline target [15]. Furthermore, we performed a number of further test simulations – increased target thickness and lateral size, varied projectile shape, fifth-order (instead of third-order) spline between Lennard–Jones and KrC potential – which corroborate our results.

3. Results

Fig. 2 gives a cross-sectional view of the penetration of the cluster into the target at a time when the cluster has reached about its maximum penetration depth. The straight 'cannon-ball-like' trajectory of the projectile is evident. Clearly, the effect on the target material is considerably more spatially constrained for larger target binding energies. For $U/U_{Ar} = 30$, Fig. 2(a), only a small crater has developed at the surface, while the material along the projectile trajectory has become amorphous or liquid. In contrast, for the small binding energy, $U/U_{Ar} = 2$, Fig. 2(c), a huge tunnel has developed along the cluster