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Velocity dependence of metal cluster deposition on an insulating surface

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Abstract. We present a detailed study of the deposition of small sodium clusters on a NaCl surface. To that end, we use a microscopic model based on the Time-Dependent Local Density Approximation (TDLDA) for electrons, coupled to classical Molecular Dynamics (MD) for ions. We discuss in particular the deposition mechanism for different initial cluster velocities and demonstrate that extremely slow velocities are necessary to ensure a cluster deposition without damaging the original cluster.

PACS. 36.40.Cg Electronic and magnetic properties of clusters – 36.40.Sx Diffusion and dynamics of clusters – 68.49.Fg Cluster scattering from surfaces

1 Introduction

Clusters on surfaces have attracted much interest over the past decade, for an overview of the development see, e.g., the sequence of ISSPIC proceedings [1–4], and the topic is still of great actual interest. The combination of materials raises many new aspects and complications in all respects, for structure as well as for dynamics. One of the basic questions is related to the dynamics of cluster deposit. When a cluster is placed on a surface, it undergoes a significant modification of its electronic structure and ionic geometry as compared to the equivalent free cluster. Such a structural modification is due to the interface energy, the electronic band structure of the substrate, and the surface corrugation. Many experimental [5–7] and theoretical works [8–13,15,16] have investigated these questions. The case of a Na cluster deposited on a NaCl surface provides a prototype example of a metallic cluster on an insulator because both materials are comparatively simple. They can be adequately described using density functional methods [8,9,11]. Besides that, the interaction with the remaining ions can be treated with pseudo-potentials [17], while any hybridization can be omitted [11]. The detailed ab initio calculations of [11] have, furthermore, shown that the substrate remains rather inert. For then, the interaction with the cluster can be treated at the level of an effective interface potential.

The calculations of [12,13] have shown that the strongly attractive interface attraction in such systems leads to stable planar configurations as ground states where electronic shell effects look different from free three-dimensional clusters. But there exist also competitive and stable three-dimensional isomers. The crystalline structure of the substrate induces a spatial modulation of the surface attraction, called corrugation [11,13]. It influences significantly the equilibrium position of the deposited cluster with respect to a Cl (more attractive) or to a Na (less attractive) site.

Up to now, the majority of theoretical investigations have dealt with clusters that are already attached to a surface. The goal of the present work is to study the process of cluster deposition itself, in real time and without adiabatic restriction for the treatment of electrons. We concentrate on the dynamics of low-energy collisions of a small neutral Na cluster with a NaCl surface. Our test case is Na_6 which has a stable planar ground-state with nearly axial symmetry as free cluster and when deposited [12]. A proper theoretical description of the system requires to account for the coupled dynamics of both electronic and ionic degrees of freedom. We treat the real-time motion of the electronic system using the Time-Dependent Local-Density Approximation (TDLDA) method numerically solved on a coordinate-space grid, while the ionic motion is described using classical Molecular Dynamics (MD) [25,26]. We present here a microscopic study of deposition of Na_6 on an insulating NaCl substrate for different initial kinetic energies of the projectile and different orientations with respect to the surface interface. A special attention will be paid to clusters with extremely low velocities, for reasons of gentle deposit. Atomic units ($\hbar = e = m_e = 1$) are used throughout the paper.

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2 Theoretical background

The Na atoms in the cluster are described in terms of their valence electrons and a singly charged ionic core. We assume that the NaCl substrate remains essentially inert [11] and can thus be taken into account as an external interface potential. The interaction amongst ions is modeled as a simple Coulomb interaction of point charges.

The valence electrons of the Na atoms in a cluster are described using density-functional theory [18]. The single-electron wavefunctions $\psi_\alpha(\mathbf{r},t)$ follow the time-dependent Kohn-Sham [19] equations

$$i\frac{d}{dt}\psi_\alpha(\mathbf{r},t) = \{-\Delta + V_{KS}\left[\mathbf{r},\rho_\uparrow(\mathbf{r},t),\rho_\downarrow(\mathbf{r},t)\right]\}\,\psi_\alpha(\mathbf{r},t), \tag{1}$$

where $\uparrow$ and $\downarrow$ arrows designate the spin of electrons, with the corresponding electron density defined as

$$\rho_\sigma(\mathbf{r},t) = \sum_{\alpha\in\sigma} |\psi_\alpha(\mathbf{r},t)|^2\,, \quad \sigma\in\{\uparrow,\downarrow\}, \tag{2}$$

and the total density is $\rho(\mathbf{r},t) = \rho_\uparrow(\mathbf{r},t) + \rho_\downarrow(\mathbf{r},t)$, respectively.

The Kohn-Sham potential V_{KS} is defined in the standard way:

$$V_{KS}(\mathbf{r},t) = V_{ext}(\mathbf{r},t) + V_{Coul}(\mathbf{r},t) + V_{xc}(\mathbf{r},t), \tag{3}$$

where the external potential V_{ext} takes into account the interaction with the surface and with the ions of the cluster. The Coulomb potential V_{Coul} is determined by solving the Poisson equation without retardation:

$$\Delta V_{Coul}(\mathbf{r},t) = -4\pi\rho(\mathbf{r},t). \tag{4}$$

The exchange-correlation potential $V_{xc}(\mathbf{r},t)$ as a functional of the spin-densities was chosen within the TDLDA framework [20] using the spin-dependent Gunnarson-Lundquist parameterization [21].

The interaction of the Na ions with the valence electrons is described by a pseudo-potential. The advantage of Na is that one can use local pseudo-potentials [22], that can be written in the smooth form of error-functions [13] as

$$V_{ps}(\mathbf{r}-\mathbf{R}) = \sum_{i=1,2}\frac{v_i}{|\mathbf{r}-\mathbf{R}|}\mathrm{erf}\left(\frac{|\mathbf{r}-\mathbf{R}|}{\sigma_i}\right) \tag{5}$$

with

$$\mathrm{erf}\left(\frac{r}{\sigma}\right) = \int_0^r \exp\left(-\frac{x^2}{2\sigma^2}\right)dx$$

which is similar to the local part of the pseudo-potential of reference [23]. The widths $\sigma_1 = 0.681a_0$ and $\sigma_2 = 1.163a_0$ and strengths $v_1 = 2.292e^2$ and $v_2 = -3.292e^2$ are chosen as in [14].

The interaction of the cluster with the surface is done in terms of a fixed effective interface potential [13,14]. This is possible because the substrate is only very little affected by the attached cluster [11]. The interface potential is derived from adjustment to the ab initio data [11]. It incorporates both the Coulomb forces and the polarization of the surface by the deposited cluster and amounts to an external one-body potential for each cluster electron V_{eff}^{el} and ion V_{eff}^{ion} (the polarization effects between the cluster ions are neglected). In the following presentation, we choose the surface parallel to the xy-plane.

The effective surface-ion potential for an atom located at position $\mathbf{R}_i = \mathbf{R}$ reads

$$V_{eff}^{ion}(\mathbf{R}) = \sum_{\alpha\in Na}\frac{1}{|\mathbf{R}-\mathbf{R}_\alpha|} - \sum_{\beta\in Cl}\frac{1}{|\mathbf{R}-\mathbf{R}_\beta|} + V_{pol}^{ion}(\mathbf{R}), \tag{6}$$

where the first two terms correspond to the Coulomb interaction with the Na^+ and Cl^- ions of the substrate. The positions of these ions are taken unchanged from the free surface.

The polarization effects are described by a polarization potential V_{pol}^{ion} of Lennard-Jones type [13,14]:

$$V_{pol}^{ion}(\mathbf{R}) = V_\perp^{ion}(Z)V_\parallel^{ion}(X,Y), \tag{7a}$$

$$V_\perp^{ion}(Z) = C^i\left(\Xi^6 - \Xi^4\right), \tag{7b}$$

$$\Xi = \frac{z_0\sqrt{\frac{2}{3}}}{Z+z_0},$$

$$V_\parallel^{ion}(X,Y) = D^i + E^i\sin(k_xX)\sin(k_yY), \tag{7c}$$

where z_0 corresponds to a minimum of $V_\perp^{ion}(Z)$ as produced by ab initio calculations [11]. The parallel component of the interface potential is periodic and accounts for the surface corrugation when moving from a Cl to a Na site [13,14].

The electronic part of the interface potential is constructed in a similar way as

$$V_{eff}^{el}(\mathbf{r}) = \sum_{\alpha\in\mathrm{Na}} V_{ps}(|\mathbf{r}-\mathbf{R}_\alpha|) - \sum_{\beta\in\mathrm{Cl}}\frac{1}{|\mathbf{r}-\mathbf{R}_\beta|} + V_{pol}^{el}(\mathbf{r}), \tag{8a}$$

$$V_{pol}^{el}(\mathbf{r}) = V_\perp^{el}(Z)V_\parallel^{el}(X,Y), \tag{8b}$$

$$V_\perp^{el}(Z) = \begin{cases} C^e\left|\zeta^6-\zeta^4\right| & \text{for } z > -z_0 + a_0 \\ V_{cutoff} & \text{for } z \le -z_0 + a_0 \end{cases}, \tag{8c}$$

$$\zeta = \frac{z_0\sqrt{\frac{2}{3}}}{|z|+z_0}, \tag{8d}$$

$$V_\parallel^{el}(x,y) = D^e + E^e\sin(k_xx)\sin(k_yy). \tag{8e}$$

The choice of V_{cutoff} in $V_\perp^{el}$ as well as the interface parameters z_0, C^i, D^i, E^i, C^e, D^e, E^e was [13]:

$$\begin{array}{lll} z_0 = 5.76a_0, & V_{cutoff} = 0.5\ \mathrm{eV}, & \\ C^e = 3.0\ \mathrm{eV}, & D^e = 1.157, & E^e = 0.629, \\ C^i = 2.56\ \mathrm{eV}, & D^i = 0.98, & E^i = -0.218. \end{array} \tag{9}$$

The molecular dynamics (MD) equations of ionic motion finally reduce to

$$\frac{d}{dt}\mathbf{P}_i = -\nabla_{\mathbf{R}_i}\left[V_{ext}(\mathbf{R}_i,t) - \int \rho(\mathbf{r},t)V_{ps}(|\mathbf{R}_i-\mathbf{r}|)d\mathbf{r} + \sum_{j\neq i}\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}\right], \tag{10a}$$

$$\frac{d}{dt}\mathbf{R}_i = \frac{\mathbf{P}_i}{M_{ion}}, \tag{10b}$$

where M_{ion} is the ionic mass.

Equations (1–4) were solved self-consistently on a coordinate space grid. Two options were used, once a fully three-dimensional (3D) grid and alternatively the cylindrically averaged pseudo-potential method [24]) where electronic densities and mean field are treated approximately as being axially symmetric thus delivering a more economic two-dimensional (2D) electronic dynamics. Benchmark calculations and first surveys were computed in full 3D. The 2D approximation has been checked to reproduce the full 3D results sufficiently well. Systematic scans and long-time asymptotics were then done with CAPS. In both, 2D and 3D, the electrons are propagated in time using the time-splitting method [27]. The Poisson equation (4) is solved by over-relaxed iteration on the grid. The equations of ionic motion (10a, 10b) were solved numerically using the standard leap-frog algorithm [29]. The full TDLDA-MD scheme and its numerical realization is described in detail in [25,26].

3 Results and discussion

3.1 Free and deposited Na_6

For the present study we have chosen the small neutral sodium cluster Na_6 which in both cases, free and deposited, has one well defined and nearly axial ground state. It was found [12,14,16] that the substrate corrugation is crucial for the precise definition of the ground state configuration of the deposited cluster. In Figure 1, we show the ground state electron density distribution and ionic configuration of the free Na_6 cluster (a) and of a Na_6 deposited on the NaCl substrate (b) in the (XY) and (XZ) planes, parallel and orthogonal to the surface. One can see that in both cases the system has mainly a planar geometry with one "extra" atom topping the five-atomic pentagonal "ring". The ground state of the system "cluster on the NaCl substrate" corresponds to the cluster deposited on top of a Cl site (see Fig. 1b) with the extra atom "facing up", in good agreement with the model calculations of [13]. For the sake of simplicity here and throughout the paper we designate the latter configuration of the cluster above the surface as "Up" configuration: the opposite situation is the "Down" geometry with the sixth atom "facing down". Furthermore, we distinguish whether the extra atom is placed above a Cl or Na site.

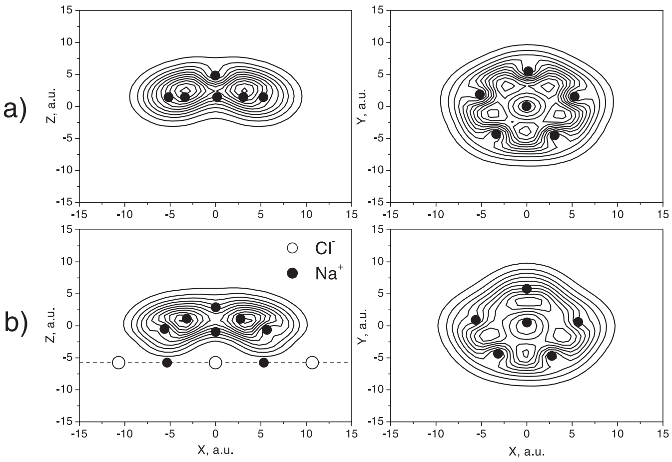

Fig. 1. Ground state configuration of (a) free Na_6 cluster and (b) of Na_6 deposited on NaCl substrate computed with the 3D code. The surface lies in the $(X$-$Y)$-plane. It is indicated by a dashed line in the lower $(X$-$Z)$-plot.

3.2 Deposition dynamics

Our study is devoted to the deposition dynamics of the cluster in real-time. We have simulated the process by solving the system of equations (1–10b). The free ground state Na_6 was initially (i.e. at $t = 0$) placed at a distance where the influence of the surface potential is negligible (i.e. initial center of mass $Z_{CM}(0) > 10a_0$) [16]. The orientation of the Na_6 ring was chosen to be parallel to the surface. The initial Center of Mass (CM) momentum points towards the surface (anti-parallel to surface normal). The corresponding initial kinetic energy is $E_{kin} = \sum_i E_{kin}^{(i)}$, where $E_{kin}^{(i)} = P_Z^2/2M_{ion}$ is the kinetic energy of a single cluster ion, i.e. we start with the same initial momenta for all the cluster ions $P_{i(Y)} = P_{i(X)} = 0$, $P_{i(Z)} = P_Z$. We consider collision energies up to a total kinetic energy of 50 eV. This corresponds to very low velocities up to about $0.2a_0$ fs and to an CM energy content of the electrons in the cluster of the order of 10^{-7} eV. Figure 2 shows the time evolution of the center of mass of the Na_6 for the case of an "Up" orientation where the center ion is placed on the surface normal on top of a Cl site (corresponding to the equilibrium configuration, see Fig. 1). Results for various initial velocities are compared. There exists obviously a deposition-threshold, i.e. a maximal initial kinetic energy below which the cluster becomes attached to the surface. For the considered orientation of Na_6 this energy threshold is about 6.9 eV. The attachment of the cluster to the substrate is accompanied by oscillations in the the effective "potential well" of the surface potential [16]. Here we should note that our model (with substrate described as an effective potential) does not take into account a possible energy transfer from the cluster to the surface excitations (in particular to the surface phonons). This coupling would induce some additional damping of these CM oscillations. The cluster-surface collisions with

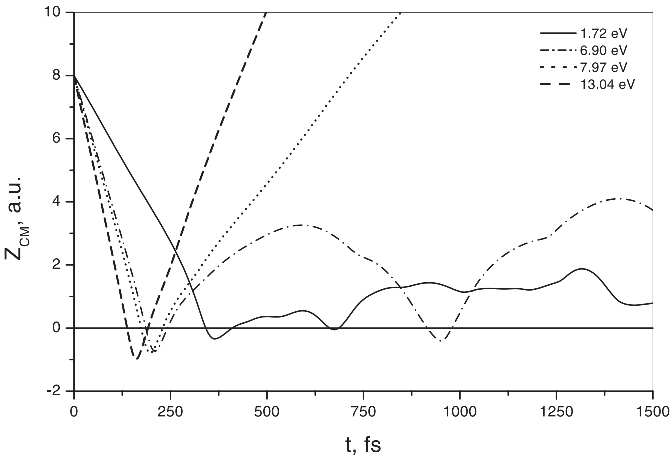

Fig. 2. Time evolution of the center of mass of the Na_6 cluster during deposition, for various initial velocities (kinetic energies), as indicated. The cluster was oriented initially parallel to the surface with the top ion facing "Up" and in direction above a Cl site. The CAPS was used.

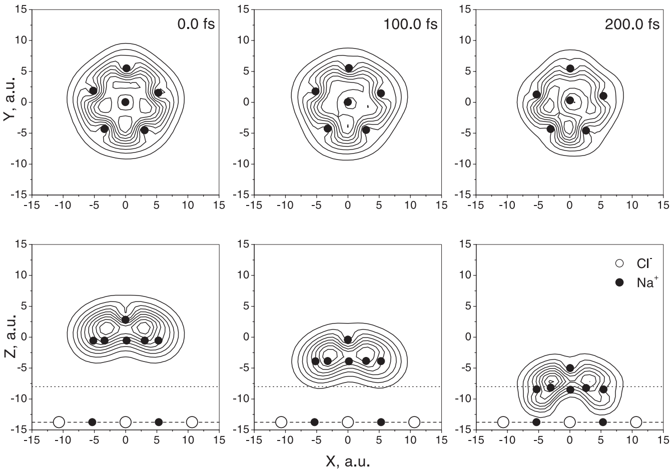

Fig. 3. Electron charge density (computed in full 3D) and ionic positions for the Na_6 cluster at different times of deposition for initial velocity $v_0 = 0.002$ (kinetic energy 6.9 eV).

an energy above the deposition threshold lead to inelastic reflection of the projectile.

In Figure 3 we show a few "snapshots" of electron density distributions and ionic configurations (in the $(X$-$Y)$ and $(X$-$Z)$ planes) for a Na_6 cluster at different times during deposition. The orientation is again "Up" and the top ion is in line with a Cl site, as in Figure 2. The initial kinetic energy of the cluster is 6.9 V, close to the deposition threshold. One can see that the collision leads to a significant cluster deformation, particularly for the electron cloud. This is produced to a large extend by corrugation. The Cl site $(X = 0)$ repels the cloud while the adjacent Na sites attract it. This excites internal degrees of freedom, especially in terms of ionic motion. One can characterize this ionic motion by the internal ionic kinetic energy or "ionic temperature" of the cluster.

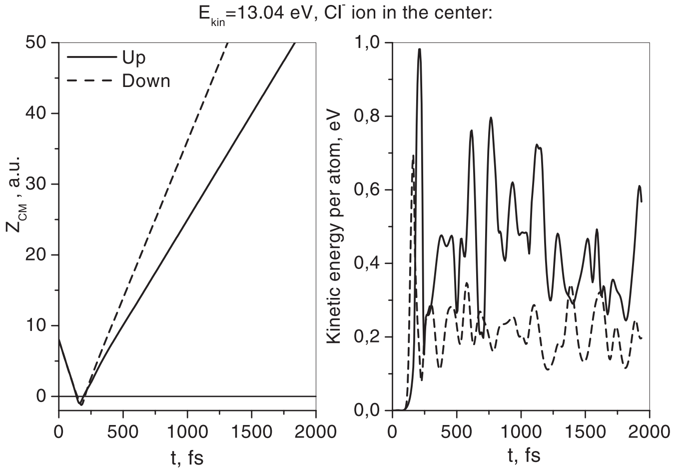

Fig. 4. Time evolution of the center of mass of the Na_6 cluster during a collision (left panel), and corresponding ionic kinetic energies per one cluster atom (right panel). Two cases with two different cluster orientations relative to the surface are displayed. The CAPS was used.

3.3 Effects of cluster orientation

It was found in [16] that the resulting internal ionic excitation depends on the initial cluster orientation. In Figure 4, we show the time evolution of the cluster CM during the Na_6 deposition for the case of deposition on the Cl substrate ion site, both for "Up" and "Down" initial orientations of the projectile (left panel). The corresponding summary of internal ionic kinetic energies is also shown (right panel) for an initial projectile kinetic energy of 13.04 eV, well above the deposition threshold. One can see, that the energy loss and, correlatively, the resulting "ionic temperature" is higher for the "Up" than for the "Down" orientation. In other words, a larger part of the initial energy is transferred to excitations of internal degrees of freedom in the "Up" case as compared to the "Down" case. This effect can be explained [16] by the damping role played by the "extra" atom in the "Down" case. In this case, the cluster-surface collision mainly results in the excitation of the degree of freedom corresponding to this sixth atom, while for the residual five-atomic "ring" the deposition occurs more softly. On the contrary, for the "Up" geometry, all the internal ionic motions are excited simultaneously.

3.4 Energy loss

For energies above the deposition threshold, the inelastic cluster reflection can be characterized by its energy loss, defined as the difference between the initial kinetic energy and the asymptotic CM kinetic energy of the reflected cluster. In upper panel of Figure 5 we plot the relative energy-loss as a function of the initial cluster kinetic energy for four different deposition configurations, i.e. both "Up" and "Down" orientations of Na_6 depositing on a Cl or a Na substrate sites, as indicated. Each curve starts at its lowest energy equal to the corresponding deposition

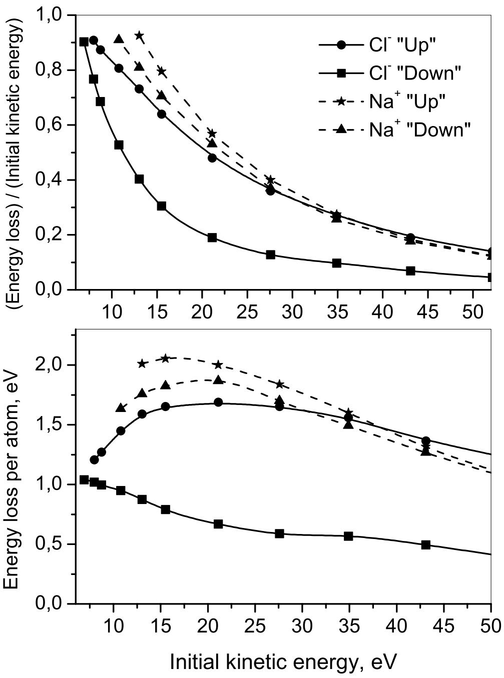

Fig. 5. Upper panel: fraction of initial kinetic energy lost during the deposition process. Lower panel: energy loss per atom (b) as a function of initial kinetic energy.

threshold. At this point about 90% of the initial kinetic energy is transferred to the internal degrees of freedom, while the residual part corresponds to the CM oscillations (see Fig. 2). The smallest deposition threshold is associated with the most "elastic" case of the "Down" orientation over a Cl site. This process has the lowest energy loss throughout all the initial projectile energies. The highest energy threshold of the cluster attachment corresponds to the most "inelastic" deposition process corresponding to an "up-looking" cluster over a Na site, which naturally results in the highest post-collision ionic temperature. The differences between "Up" and "Down" configurations are smaller for a Na site than for a Cl site. This may be explained by the fact that the repulsion from the Cl site makes more effect if it hits the distinguished top ion.

The lower panel of Figure 5 shows the net energy loss per cluster atom as function of initial kinetic energy. One should compare the obtained values with the typical binding energy per atom defined as $E_{\mathrm{B}}/N = E_{\mathrm{at}} - E_N/N$, where E_N is the total energy of a neutral free cluster with N atoms and E_{at} is the energy of one single Na atom. Our LDA calculations yield for the Na_6 cluster a binding energy per atom of $E_{\mathrm{B}} = 0.3$ eV. This is significantly lower than the energy per cluster atom obtained in the collision with the surface. For example, at 12 eV total kinetic energy (2 eV per atom) one observes about 1 eV energy loss per atom which means about 1 eV excitation energy per atom in the cluster to be compared to the binding of 0.3 eV per atom. So far, we can conclude that due to the significant excitation of the ionic degrees of freedom the inelastic reflection of a cluster with a high probability leads to its further destruction. This assumption is in agreement with our calculations of the post-collision ionic motion.

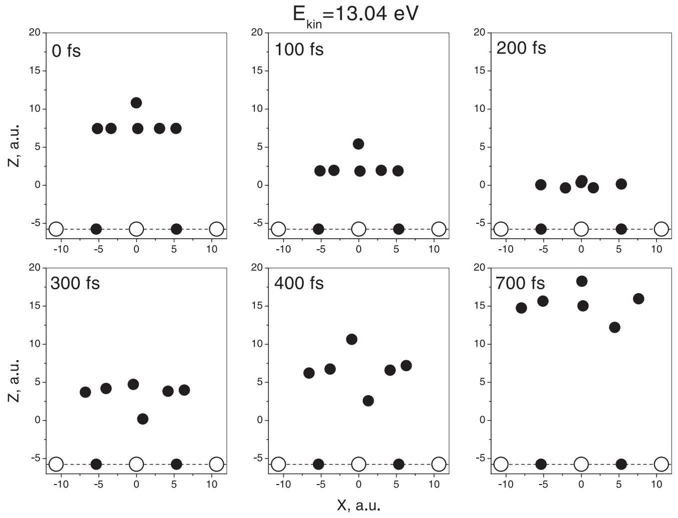

Fig. 6. Time evolution of the Na_6 cluster ions deposition process with initial kinetic energy 13.04 eV for the orientation "Cl Up".

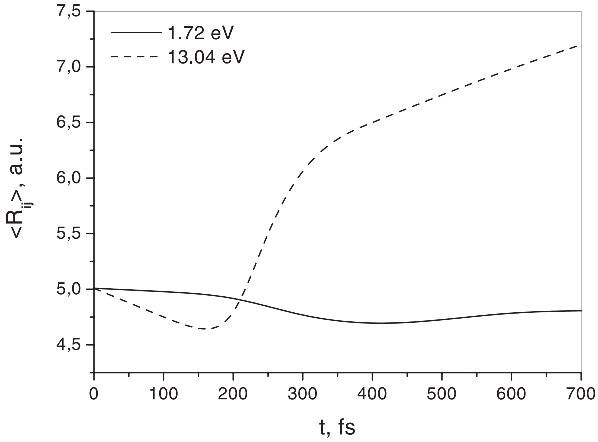

Fig. 7. Average interatomic distances for the orientation "Cl Up" and for two initial kinetic energies, as indicated.

3.5 Asymptotic behavior

Figure 6 shows "snapshots" of ionic motion in Na_6 during its deposition on the Cl site with "Up" orientation and initial kinetic energy of 13.04 eV (i.e. above deposition threshold). One can see that at time 700 fs the atoms of the reflected cluster are practically dissociated.

The averaged interatomic distances for two kinetic energies of 1.72 eV (below deposition threshold) and 13.04 eV (above the threshold) are plotted in Figure 7. The case above threshold goes clearly into steady total dissociation of the clusters while the very gentle case far below threshold stays nicely bound with some small residual oscillations. This picture is a complementing illustration for the violent dissociation in cases above threshold. And it substantiates our previous conclusion that extremely slow velocities are necessary for cluster deposition without damaging the original cluster.

4 Conclusions

We have presented a theoretical study of the low-energy deposition of small neutral Na clusters on an insulating NaCl surface. The description was based on self-consistent calculations of real-time dynamics of electronic and ionic subsystems of the projectile in the framework of a time-dependent local-density approximation non-adiabatically coupled to ionic molecular dynamics. The interaction of the cluster with the substrate was described using an effective interface potential incorporating both the Coulomb forces and the polarization of the surface by the deposited cluster accounting also for the surface corrugation. It was demonstrated that there exists a threshold for the initial kinetic energy below which a cluster is attached to the surface. The attachment process is sensitive to the initial cluster orientation with respect to the surface as well as whether the deposition occurs over a Cl or a Na site of the substrate lattice. In particular, the kinetic energy loss of the projectile, and, as a result, its post-collision behavior depend strongly on the collision conditions. Low-energy deposition ends up with center of mass oscillations in the vicinity of the final equilibrium position. Initial kinetic energies above the deposition threshold results in inelastic reflection of the cluster. The amount of absorbed energy and internal ionic motion is usually so large that the whole cluster dissociates while departing away from the collision zone.

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