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DIFFUSION ON Cu SURFACES

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Introduction

Understanding surface diffusion is essential in understanding surface phenomena, such as crystal growth, thin film growth, corrosion, physisorption, and chemisorption. Because of its importance various experimental and theoretical efforts have been directed to understand this phenomena. Field Ion Microscope (FIM) has been the major experimental tool for studying surface diffusion. FIM have been employed by various research groups to study surface diffusion of adatoms. Because of limitations of the FIM such studies are only limited to a few surfaces; nickel, platinum, aluminum, iridium, tungsten, and rhodium (4, 5). From the theoretical standpoint, various atomistic simulations are performed to study surface diffusion. In most of these calculations the Embedded Atom Method (EAM) of Daw and Baskes(2) along with the molecular static (MS) simulation are utilized. The EAM is a semi-empirical approach for modeling the interatomic interactions. The MS simulation is a technique for minimizing the total energy of a system of particles with respect to the positions of its particles.

One of the objectives of this work is to develop the EAM functions for Cu and use them in conjunction with the molecular static (MS) simulation to study diffusion of a Cu atom on a perfect as well as stepped Cu(100) surfaces. This provide a test of the validity of the EAM functions on Cu(100) surface and near the stepped enviroments. In particular, we construct a terrace-ledge-kink (TLK) model (figure 1) and calculate the migration energies of an atom on a terrace, near a ledge site, near a kink site, and going over a descending step. We have also calculated formation energies of an atom on the bare surface, a vacancy in the surface, a stepped surface, and a stepped-kink surface. Our results are compared with the available experimental and theoretical results.

Methodology

Pair potentials suffer at least from two major problems. Cauchy pressure C_{11}-C_{12}=0 and single vacancy formation energy is equal to the cohesive energy $E_{1v}=E_c$. For a metal $C_{11}\neq C_{12}$ and $E_{1v}\neq E_c$. To overcome these and other shortcomings, the EAM potential is developed for Cu. In the EAM, energy of each atom is approximated with sum of the embedding and two body contributions,

$$E_i=F_i(\rho_i)+.5\sum \phi(r_{ij}), \qquad (1)$$

where$F_i(\rho_i)$ is the embedding energy of atom i which can be interpreted as the energy that is required to embed an atom into the electronic charge created by the other atoms, ρ_i is the charge density at site i, $\phi(r_{ij})$ is the two body potential between atoms i and j, and r_{ij} is the separation distance between atoms i and j. ρ_i is approximated with the superposition of atomic charge densities(1, 2). Functional forms are considered for F and ϕ and their parameters are determined by fitting to the bulk properties of crystalline solid (1, 2).

In our calculations, we have employed two sets of EAM potentials one developed by us(2) and the other one developed by Adams et.al.(3). We have utilized the above EAM potentials along with the MS simulation to calculate formation energies of an atom on the surface, a vacancy on the surface, stepped surface, and stepped kink surface. We have also calculated migration energies of an atom on the bare surface, near a ledge, near a kink, and over a descending step.

Results

a) Adatom formation and migration energies

Our lattice is a slab of 12 parallel layers with 144 atoms per layer. An atom is placed on the surface layer and the formation and migration energies of the adatom are calculated from the following formulas(4, 5),

$$E^f_{1a}=E(N+1,1) - E(N,0)+E_S \quad , \qquad (2a)$$
$$E^m_{1a}=E_{sad} - E_{min} \quad , \qquad (2b)$$

where E^f_{1a} is the formation energy of an adatom, E(N+1,1) is the total minimized energy of the lattice of N atoms and one adatom, E(N,0) is the minimized energy of the lattice of N atoms, E_S is the sublimation energy(negative of cohesive energy), E^m_{1a} is the migration energy of an adatom, E_{sad} is the minimum total energy of the system with adatom at the saddle point , and E_{min} is the minimum total energy of the system with adatom in a lowest energy binding site. Our results for E^f_{1a}, E^m_{1a}, and activation energy $Q_{1a}=E^f_{1a} + E^m_{1a}$ are .71ev, .48ev, and 1.19 ev, respectively.

b) Vacancy formation and migration energies

A vacancy is created in the surface of the slab in part (a) and formation E^f_{1v} and migration E^m_{1v} energies of the vacancy are calculated from the following formulas (4, 5),

$$E^f_{1v}=E(N-1,1) - E(N,0) -E_S \quad , \qquad (3a)$$
$$E^m_{1v}=E_{sad} - E_{min} \quad , \qquad (3b)$$

where E(N-1,1) is the minimized energy of the lattice of N atoms and one vacancy. Our results for E^f_{1v}, E^m_{1v}, and Q_{1v} are .59 ev, .35 ev , and Q_{1v}=.95 ev , respectively.

c) Formation energies of steps

A step similar to one in figure 1 is constructed and its formation energy is calculated using the following formula (4, 5),

$$E_{step} = E - N_1 E_u + N E_S \quad , \qquad (4)$$

where E is the total minimized energy of the system of N atoms with step, N1 is the total numbers of atoms of upper and lower terraces, and Eu is the surface energy. Our results for the formation energies of steps with and without kink are .11 ev/A and .05 ev/A , respectively.

d) Migration energies of an atom for various moves

Migration energies of an atom for various moves on a stepped surface(shown in figure 1) are calculated using formula 2b. Our results for migration energies of moves

a, b, c, d, e, f are .485 ev, .246 ev, .507 ev, .834 ev, .522 ev, .and 355 ev, respectively.

e) Migration energies of an atom on bare surfaces

Migration energies of an atom on Cu(100), Cu(110), Cu(111) are calculated using formula 2b. Our results are E^m_{1a}=.48 ev, $E^m_{1a}(110)\|$=.23 ev, $E^m_{1a}(110)\perp$=.30 ev, and $E^m_{1a}(111)$=.026 ev for (100), (110), and (111) surfaces.

Summary and conclusion

a) Vacancy diffusion is dominant diffusion on Cu(100) surface. This is in agreement with another simulation results.

b) Migration energies of an adatom follows the following trend, $E^m_{1a}(100) > E^m_{1a}(110) > E^m_{1a}(111)$. This is consistent with other simulations and experiments.

c) The formation energies of an adatom, a vacancy, a step without kink, a step with kink are calculated. The trend is consistent with other simulations.

d) Migration energy of an atom along the ledge on a Cu(100) stepped surface is smaller than its corresponding value on a bare Cu(100) surface. This is consistent with another simulation.

e) Migration energy of an adatom over a descending step is slightly larger than its corresponding value on a bare Cu(100) surface. This result is in qualitative agreement with another computer simulation.

References

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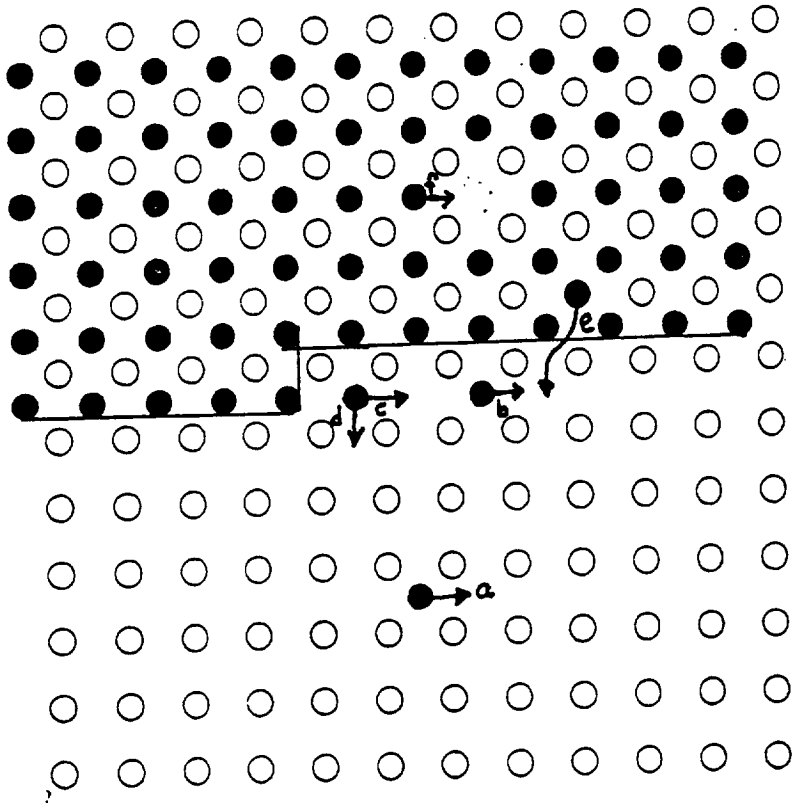

Fig. 1