Self-diffusion of small Ag, Cu and Ni islands on fcc(111) surfaces: an application of SLKMC-II

Syed Islamuddin Shah, Giridhar Nandipati, Abdelkader Kara, Talat S. Rahman

University Of Central Florida

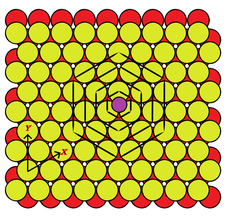
Introduction

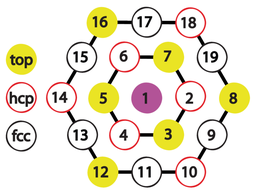
We report the development of a pattern-recognition scheme that takes into account both fcc and hcp adsorption sites in performing self-learning kinetic Monte Carlo (SLKMC-II) simulations on the fcc(111) surface. In this scheme, the local environment of each under-coordinated atom is uniquely identified by grouping the fcc and hcp sites and the top-layer substrate atoms around it into hexagonal rings. As simulation progresses, all possible processes – including shearing, reptation and concerted gliding, which may involve fcc-fcc, hcp-hcp and/or fcc-hcp moves are automatically found, and their energetics calculated on the fly . We present results of application of this new pattern-recognition scheme to the self-diffusion of M9/M(111), where M = Cu, Ag or Ni.

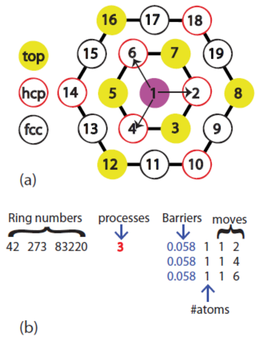
Self Learning KMC [a]

Pattern Recognition

- Used to collect information about local environment of cluster atoms
- Unique Binary number generated based on the local neighborhood: a base ten number is associated with each shell as shown below.
- Only 2 of the considered shells are shown in figure
- Each event
  - is identified based on local environment.
  - involves a central atom and other atoms in the cluster
  - involves a central atom moving to neighboring vacancy
  - is accompanied by the motion of any other atom or atoms in its surrounding shells







Ring #	Binary #	Decimal #
1	010101	42
2	000100010001	273
3	00101000101000101000	83220

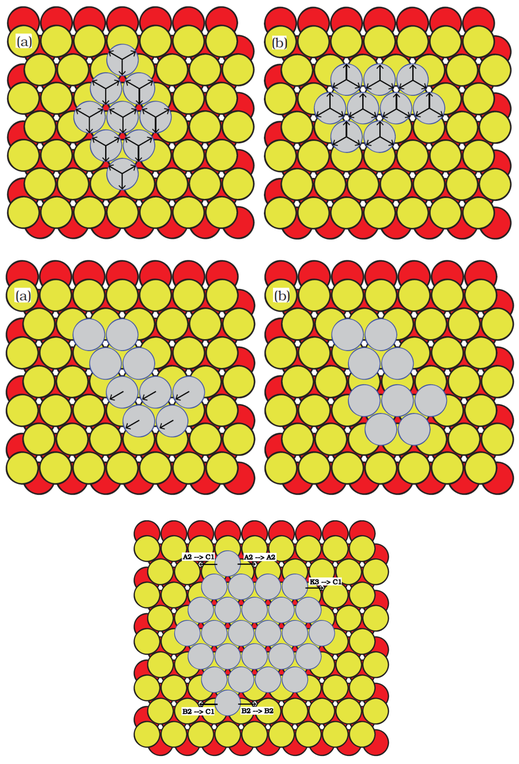
Activation Barriers

- EAM [b] potential to calculate activation energy barriers.
- Drag Method – central atom is moved in steps towards aimed final position.
- Coordinate of central atom along direction of motion fixed
  - all other degrees of freedom of central atom are relaxed
  - all degrees of freedom of all the other atoms are relaxed
- Novel single atom as well as multi-atom processes are revealed.

Symmetry Operations

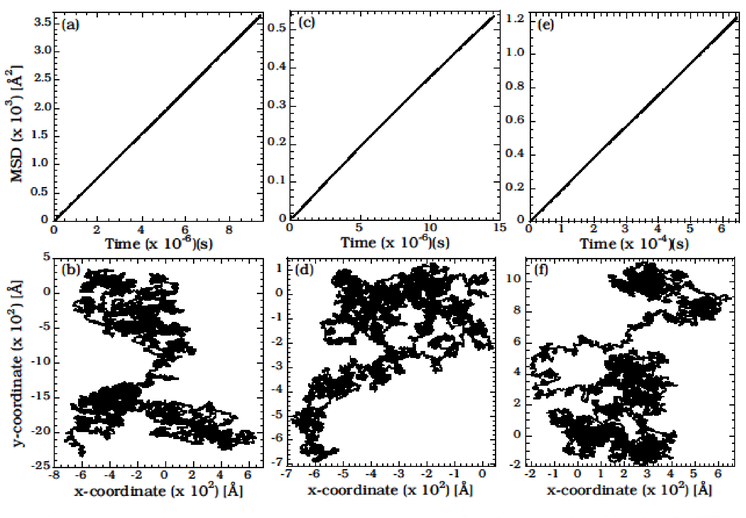
- Rotation 120^0 and 240^0 clock wise
- Mirror Reflection
- Mirror Reflection and Rotation 120^0
- Mirror Reflection and Rotation 240^0

Key processes and their barriers



Processes	Ag	Ni
Concerted	.420	.530
A(B)2->C1	.300(.350)	.400(.538)
A(B)2->A(B)2	.260(.330)	.320(.440)
C1->A(B)2	.070(.130)	.040(.180)
KA(B)3->C1	.462(.550)	.730
A(B)2->K3	.250(.330)	.280(.318)
KA(B)3->A(B)2	(.540)	
KA(B)4->C1	(.747)	

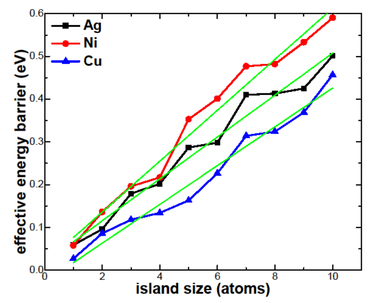
Center of Mass Trajectories and MSD

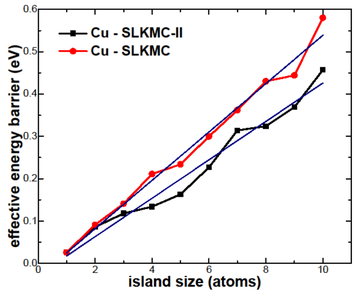


Mean square displacements and center of mass trajectories for Cu(a & b), Ag(c & d), Ni(e & f) @ 500K

Results

Size dependence of effective energy barriers





Size	E_{eff} (eV)		
	Ag	Ni	Cu
1	0.059	0.058	0.027
2	0.096	0.136	0.086
3	0.179	0.196	0.118
4	0.202	0.217	0.134
5	0.287	0.353	0.163
6	0.298	0.401	0.227
7	0.410	0.477	0.314
8	0.413	0.482	0.324
9	0.425	0.533	0.369
10	0.501	0.590	0.457

Size	E_{eff} (eV)	
	SLKMC-II	SLKMC
1	0.027	0.026
2	0.086	0.091
3	0.118	0.141
4	0.134	0.211
5	0.163	0.234
6	0.227	0.300
7	0.314	0.362
8	0.324	0.430
9	0.369	0.444
10	0.457	0.580

Conclusions

- New pattern recognition scheme includes both fcc and hcp sites on the fcc (111) surface.
- Different types of processes including concerted motion from fcc-to-hcp (hcp-to-fcc) were found using the Drag Method.
- Effective energy barrier increases with cluster size, for small clusters, as 0.049, 0.060 & 0.045 eV/atom for Ag, Ni and Cu respectively.
- Diffusion coefficient decreases with island size and increases with temperature for small islands.
- Comparison of the results for small Cu islands with those obtained from simulations (SLKMC I) without hcp sites in the pattern recognition scheme show trends that can be explained.

Acknowledgements:

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[a] *O. Trushin et al PRB 72, 115401 (2005)* [b] *M. I. Basks And M. S. Daw PRB 33, 7983(1986)*