50-я Международная Тулиновская конференция по физике взаимодействия заряженных частиц с кристаллами

МОДИФИКАЦИЯ ЯНУСОПОДОБНЫХ ДВУХКОМПОНЕНТНЫХ КЛАСТЕРОВ ПОД ДЕЙСТВИЕМ ЧАСТИЦ Ar_1 И Ar_{13} НИЗКИХ ЭНЕРГИЙ

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25–27 Мая 2021, МГУ им. М. В. Ломоносова, Москва, Россия

Outline

- ***Review***
- ***Prologue*** : MD simulation of Cu-Cu, Cu-Au, Cu-Bi, Ni-Al Janus-like clusters under argon particle impacts from 2013.
- The MD model - details.
- The 100-500 ps kinetics and final magnitudes of geometric characteristics, potential energy, temperature and sputtering yields of the Ni-Al, Cu-Au and Cu-Bi Janus-like nanoclusters under up to1.0 keV Ar and Ar_{13} impacts.
- The influence of bombarding regimes on the intensity of core-shell structure formation in the Ni-Al, Cu-Au and Cu-Bi Janus-like cluster.
- ***Epilogue*** : conclusion and outlook.

Review

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Prologue : MD simulation of Cu-Cu, Cu-Au, Cu-Bi, Ni-Al Janus-like clusters under argon particle impacts from 2013

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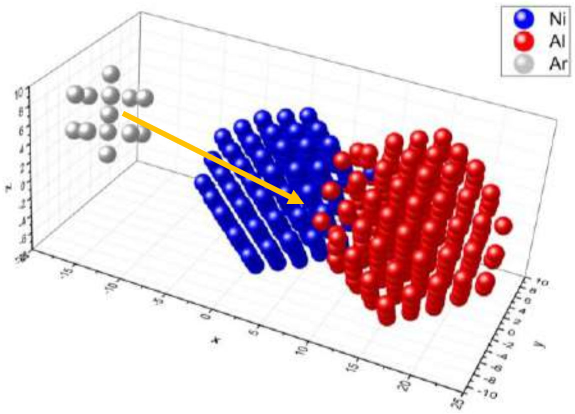
The MD model

Initial Janus-like Ni-Al cluster, Ar_{13} impact cluster



The enthalpy of mixing:

$$\Delta H_{mix} = E_{rand} - C_1 \cdot E_1 - C_2 \cdot E_2 \ ;$$

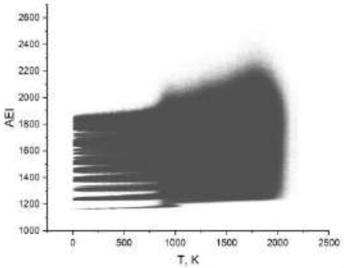
E_1 and **E_2** - the cohesive energies of elements 1 and 2 in pure states;
C_1 and **C_2** - the atomic fractions in the alloy;
E_{rand} – the cohesive energy of a random alloy;

Details

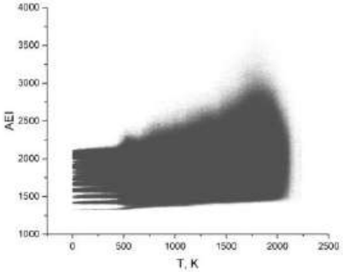
- 195Ni+195Al atoms = Ni-Al cluster;
- Ni(Al)-Ni(Al): Ackland + BM potentials;
- Ar-Ar: HFDTCS1 + BM potential;
- Ar-Ni(Al): ZBL potential;
- Ni, Al, Cu, Au mono-component cluster parts - non-ideal truncated octahedrons with hexagonal {111} and square {100} faces, fcc internal part; Bi mono-component cluster part has a shape close to sphere with surface fragments of the rhombic dodecahedron, bcc internal part; Ar13– icosahedrons;
- Hmix Ni–Al: **−22** kJ/mol, Cu–Au: **−9** kJ/mol, Cu-Bi: **15** kJ/mol;
- The energy dissipation procedure 150 ps, the temperatures o f relaxed Janus-like Ni-Al, Cu-Au, Cu-Bi clusters did not ex ceed 0.01K;
- Ar and Ar_{13} impact energies up to 1.0 keV, 200 tests, cluster e volution for 100 or 500 ps;
- The authors' MD code, Verlet algorithm, time step <0.5 fs. The OpenMP and MPI technologies, the C/C++ environment, computer systems with distributed and shared memory.

MD simulated melt points of 195 atom Ni, Al, Cu, Au and Bi clusters. AEIs (Atomic Equivalence Indexes) method

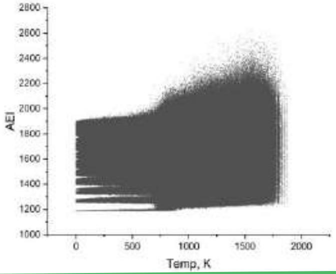
Ni, 870 K (1726 K)



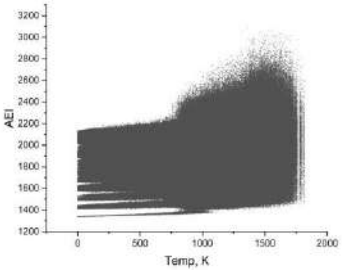
Al, 550 K (933,5 K)



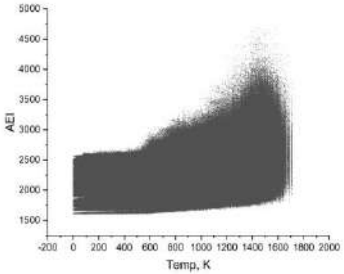
Cu, 750 K (1356,6 K)



Au, 840 K (1337,3 K)



Bi, 350K (544,5 K)



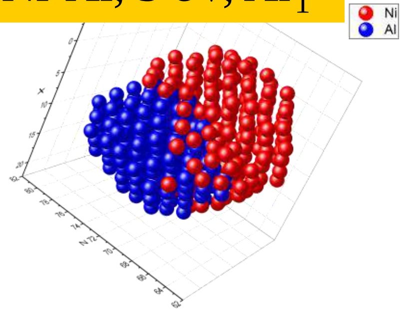
AEIs method

$$\sigma_i(t) = \Sigma_j |r_i(t) - r_j(t)|,$$

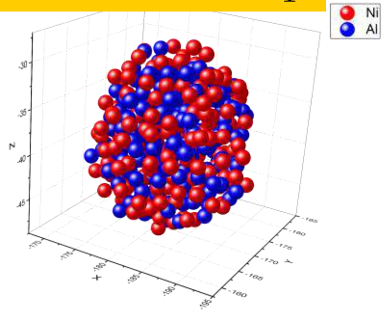
where ri (t) is the position of i-th atom at time t [1].

Appearance of the Ni-Al clusters at 5, 25 and 100 eV Ar_1 and Ar_{13} impacts after 500 ps evolution

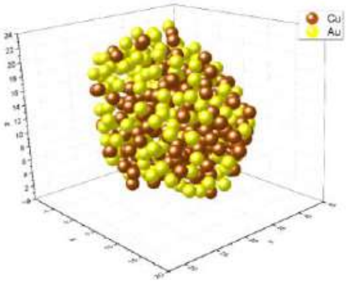
Ni-Al, 5 eV, Ar_1



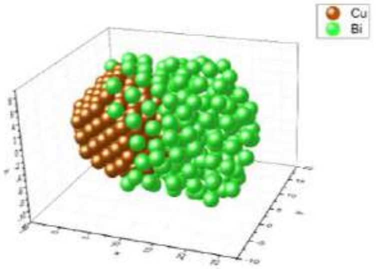
Ni-Al,100 eV, Ar_1



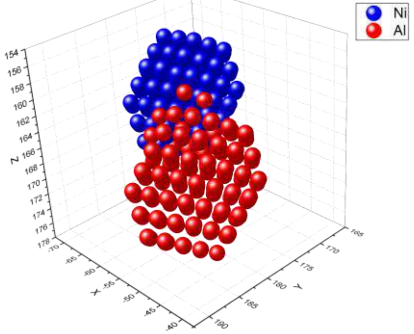
Cu-Au, 300 eV, Ar_1



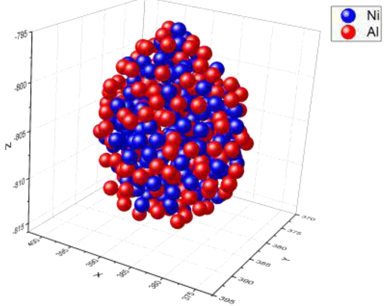
Cu-Bi, 300 eV, Ar_1



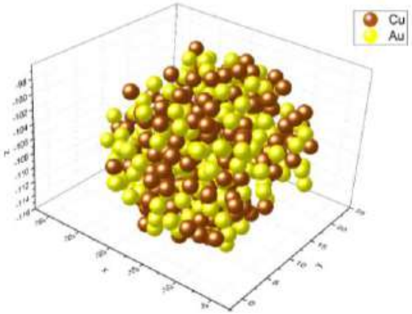
Ni-Al, 5 eV, Ar_{13}



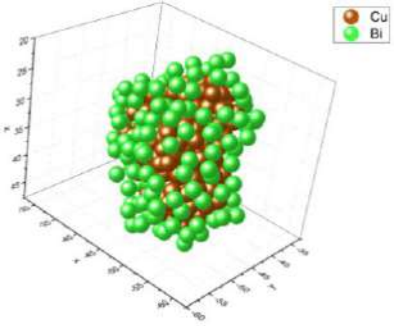
Ni-Al,100 eV, Ar_{13}



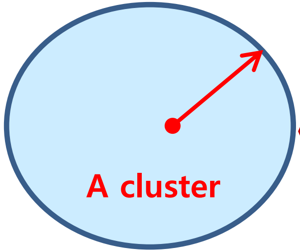
Cu-Au, 300 eV, Ar_{13}



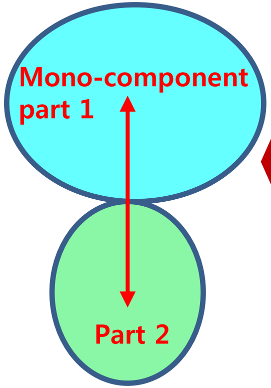
Cu-Bi, 300 eV, Ar_{13}



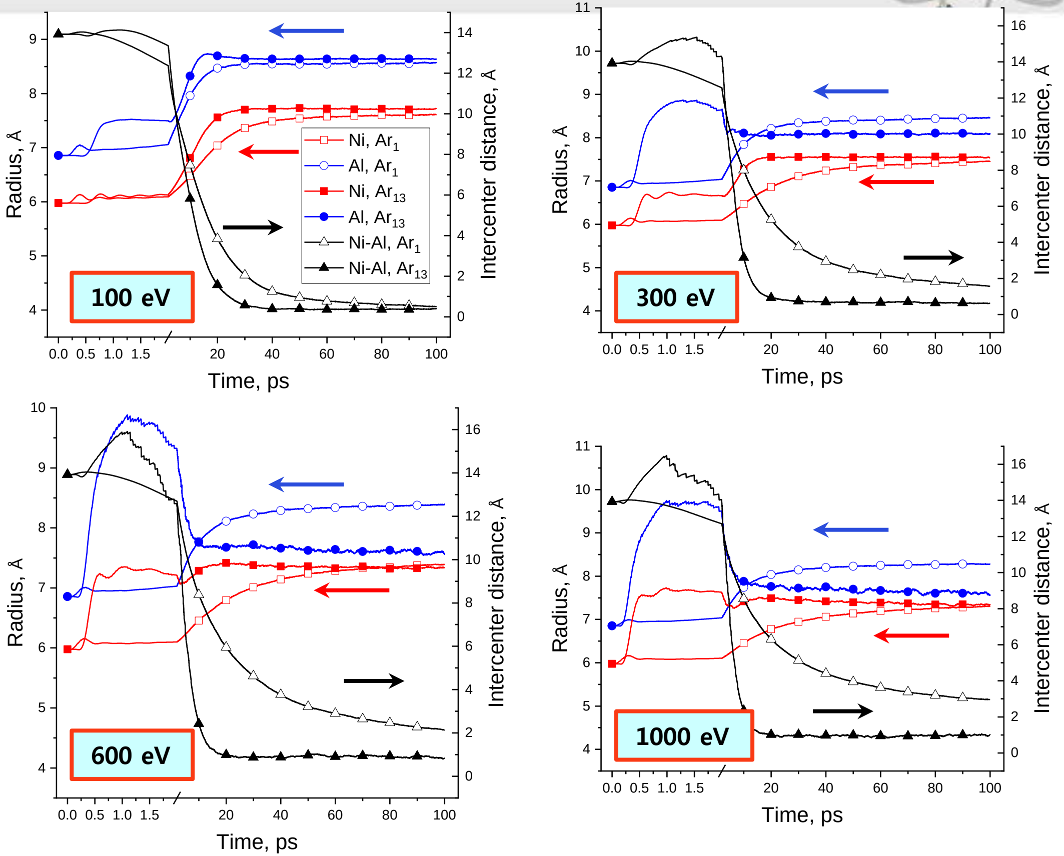
The evolution of Ni-Al clusters' radii and intercenter distances at different impact energies



The **average radius** is the mean distance from all unsputtered atoms of one type to the mass center of the same mono-component part.

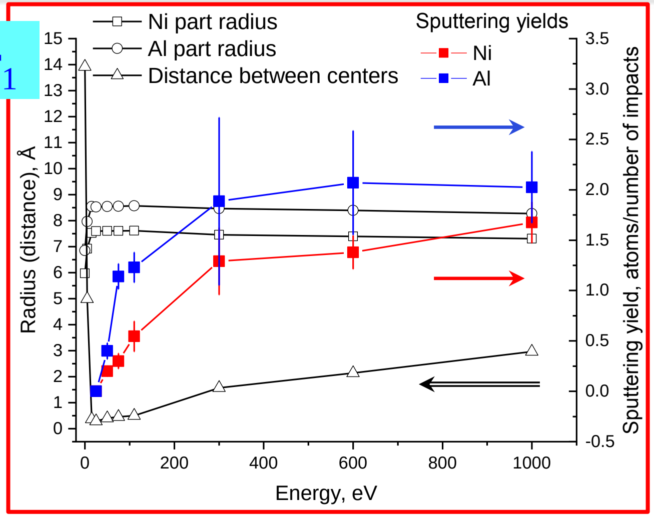


The **intercenter distance** is the distance between the mass centers of the mono-component parts.

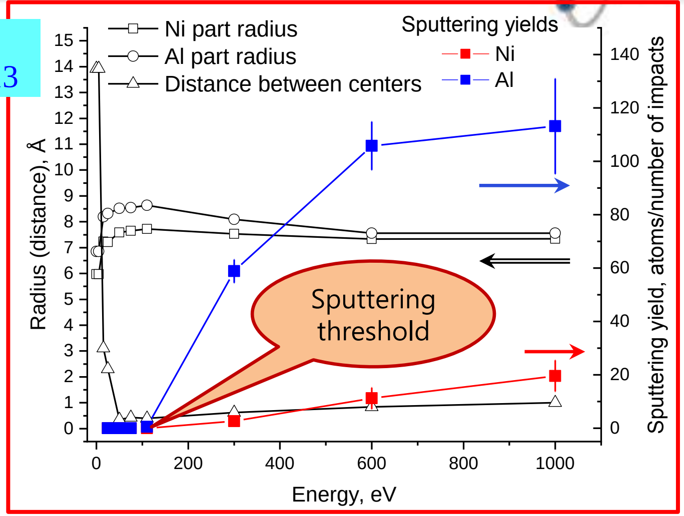


Radii of mono-component parts and intercenter distances after 100 ps

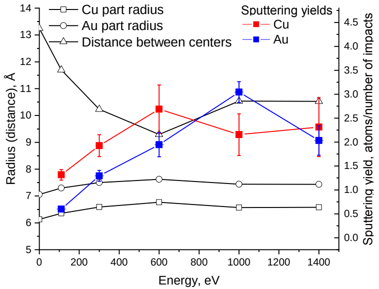
Ni-Al, Ar_1



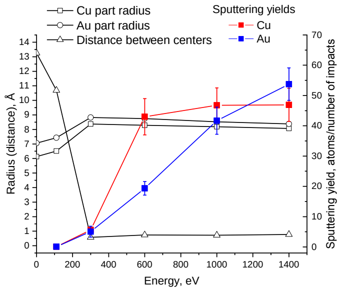
Ni-Al, Ar_{13}



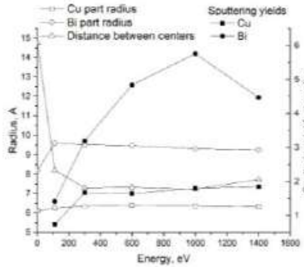
Cu-Au, Ar_1



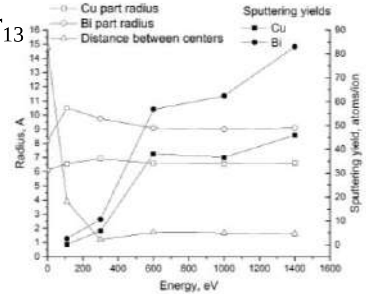
Cu-Au, Ar_{13}



Cu-Bi, Ar_1

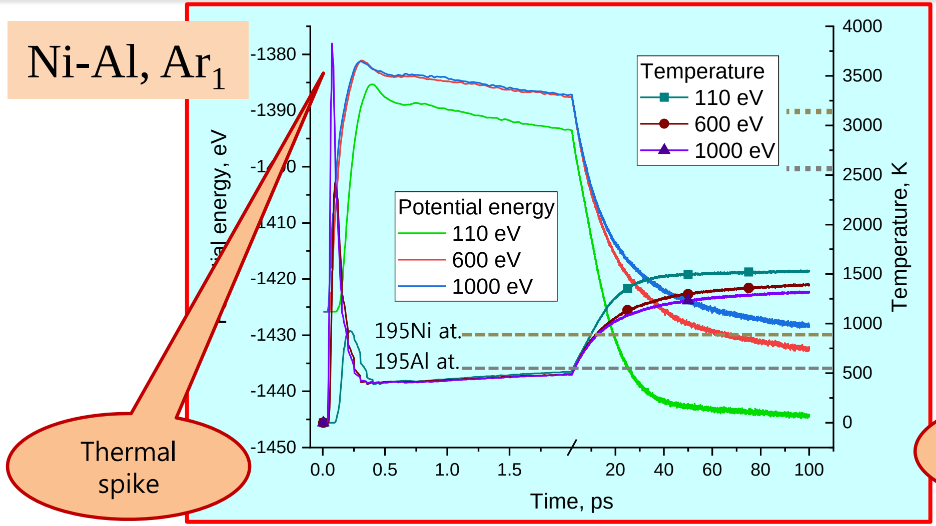


Cu-Bi, Ar_{13}

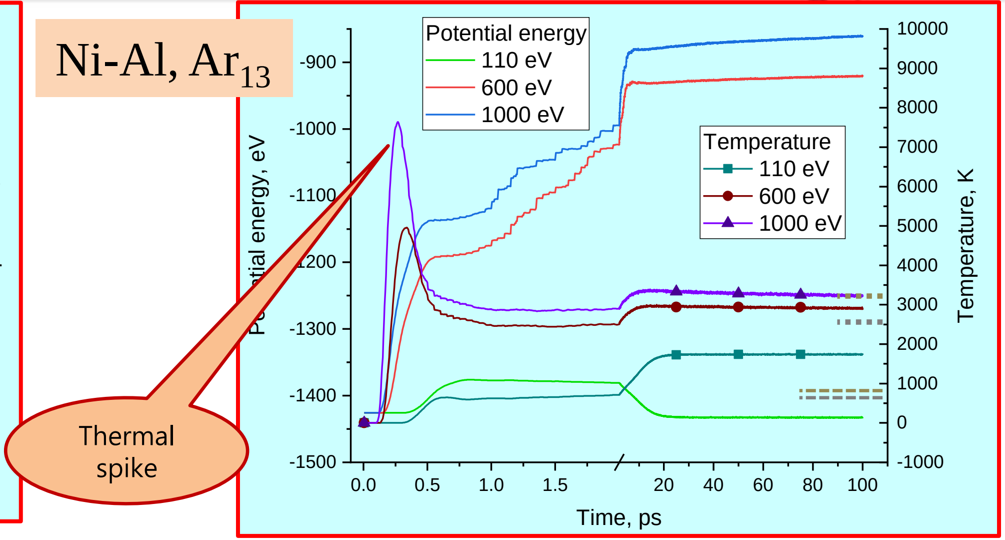


Evolution of the potential energy and temperature of the clusters at different impact energies and projectiles

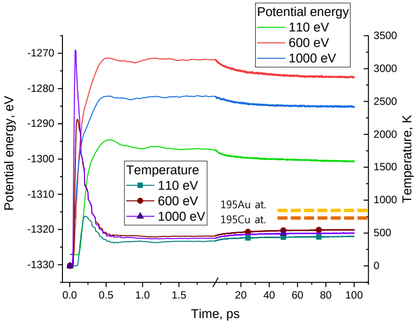
Ni-Al, Ar_1



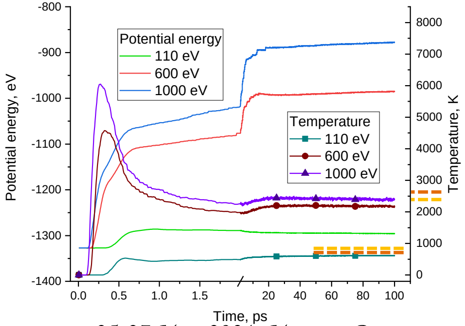
Ni-Al, Ar_{13}



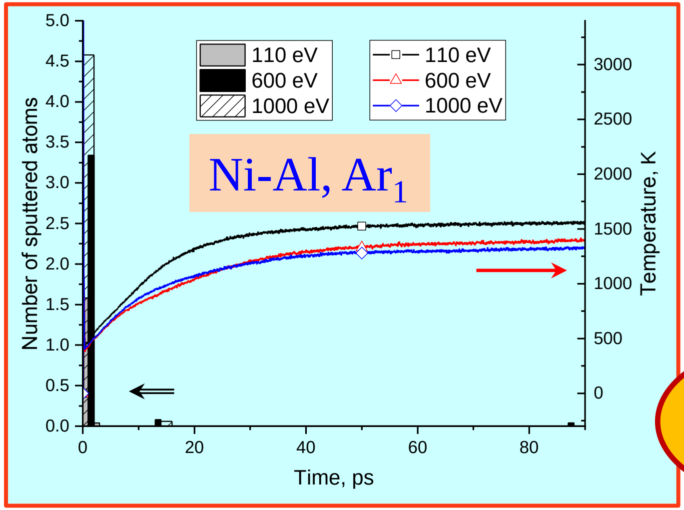
Cu-Au, Ar_1

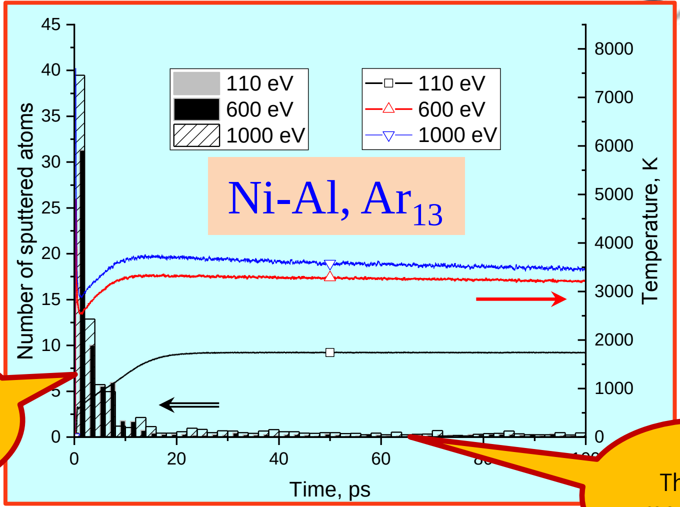


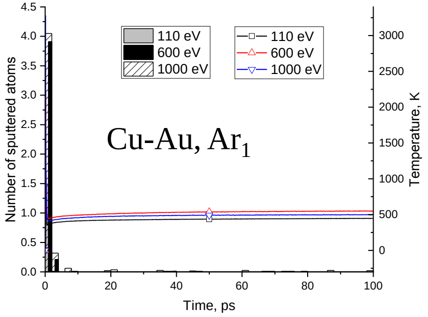
Cu-Au, Ar_{13}



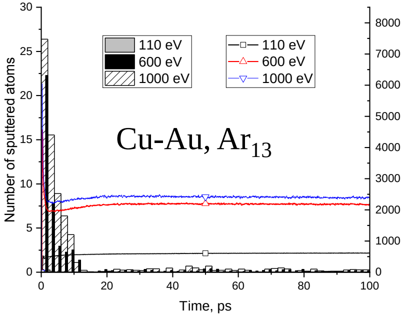
Temperature and sputtering yield kinetics of Ni-Al clusters at Ar_1 and Ar_{13} impacts

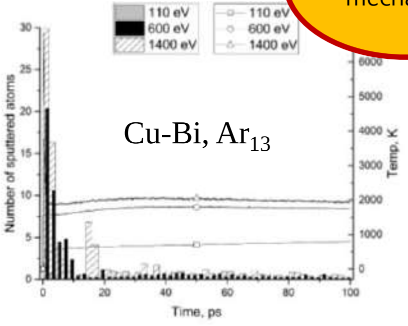






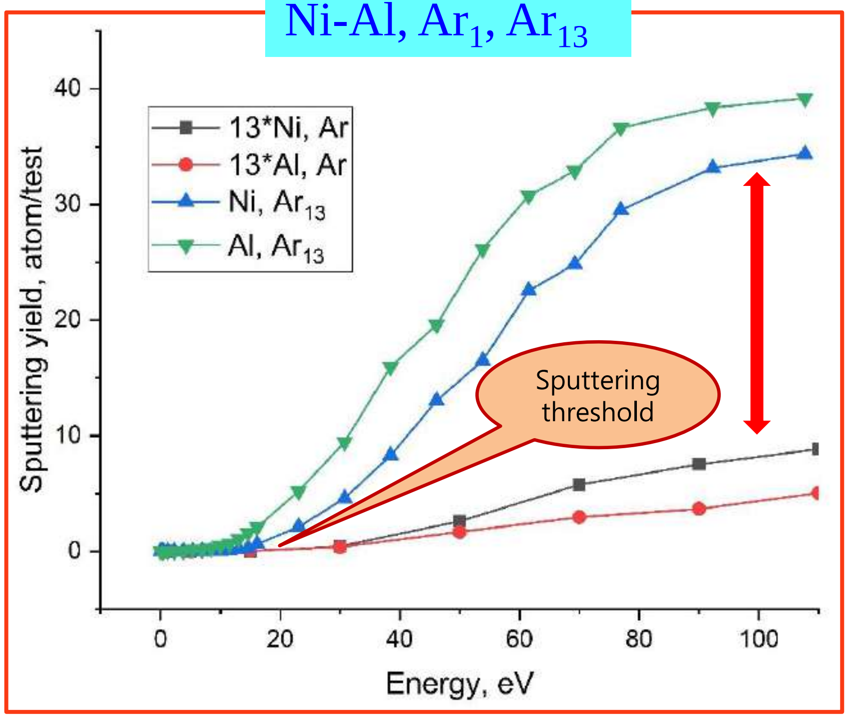
	Boil, K MD, clust.	Boil, K Table	Coh, eV MD, bulk
Ni	3200	3005	4.04
Al	2500	2792	3.15
Cu	2530	2840	3.47
Au	2330	3129	3.75



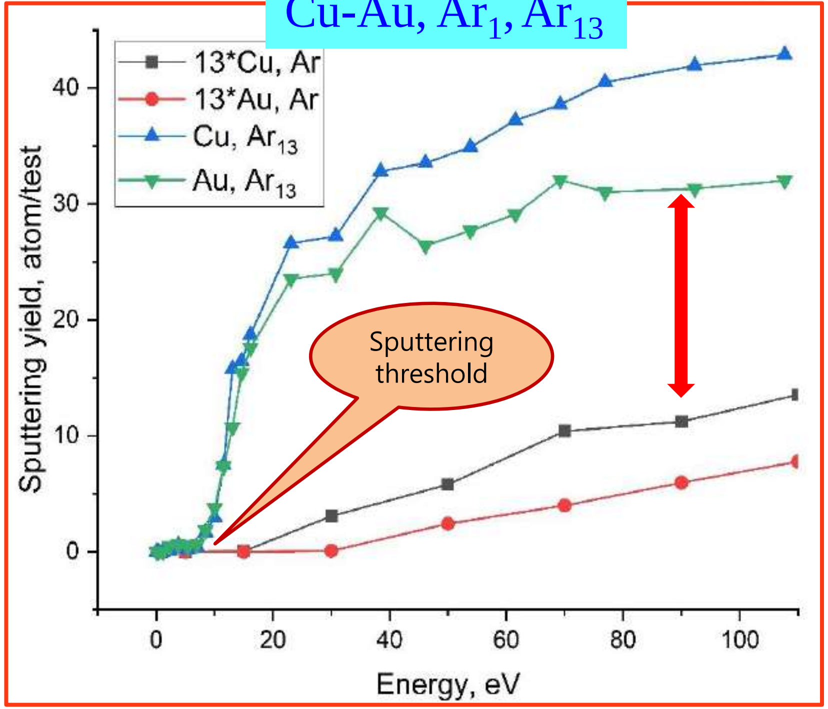


Synergistic sputtering effect in the Ni-Al and Cu-Au clusters at Ar_1 and Ar_{13} impacts

Ni-Al, Ar_1, Ar_{13}



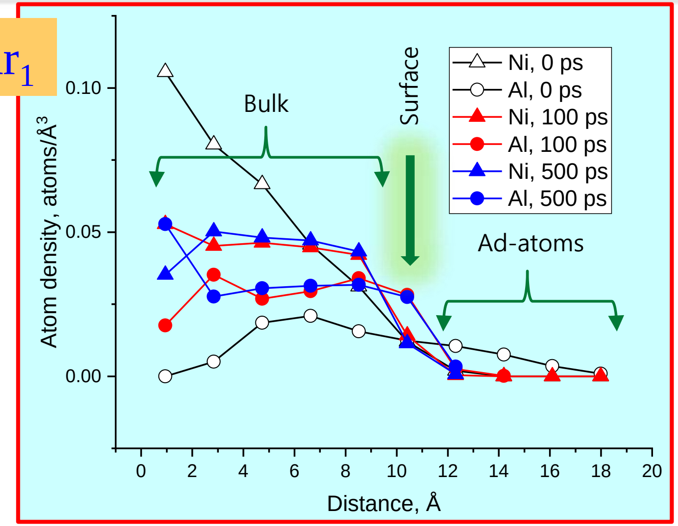
Cu-Au, Ar_1, Ar_{13}



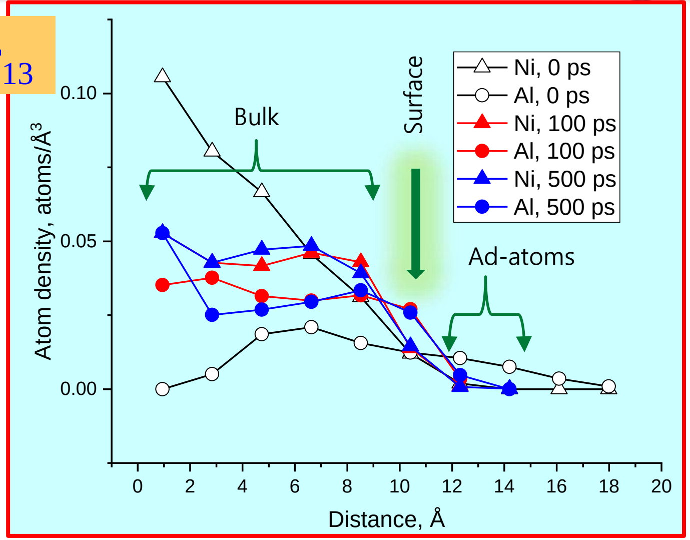
The abscissa axis – the energy per one Ar atom

Spherical distributions of atomic densities of the mono-component parts in the clusters at the 100 eV impact energy

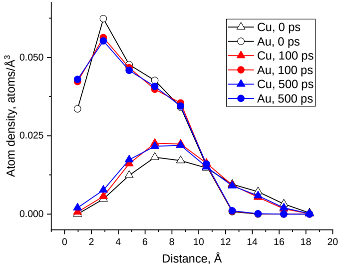
Ni-Al, Ar_1



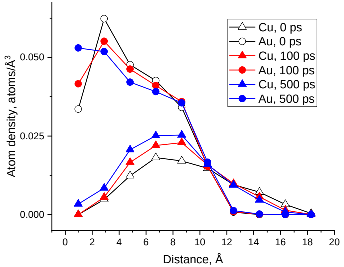
Ni-Al, Ar_{13}



Cu-Au, Ar_1

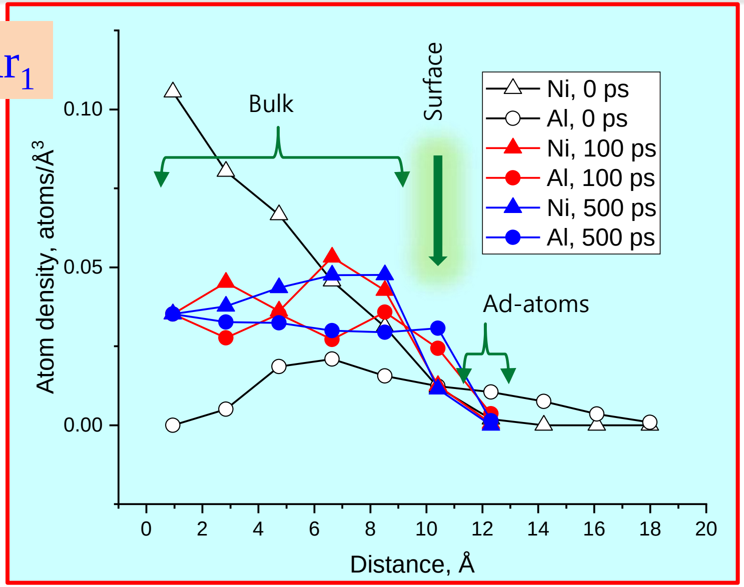


Cu-Au, Ar_{13}

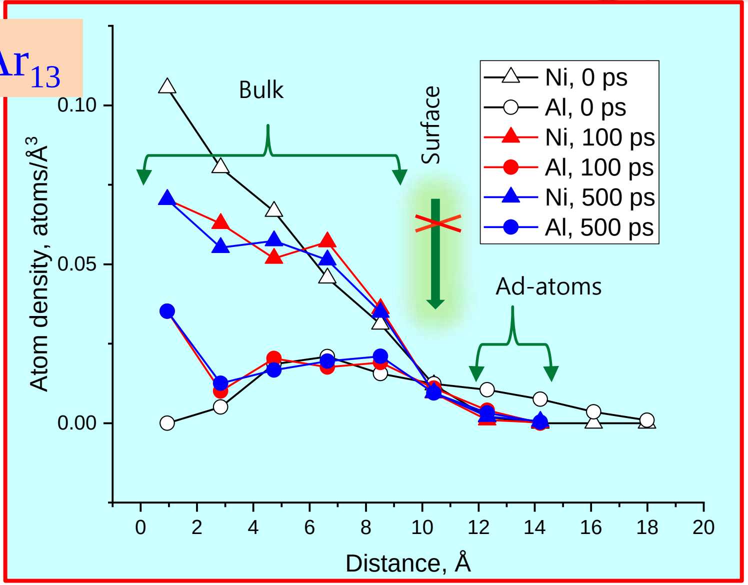


Spherical distributions of atomic densities of the mono-component parts in the clusters at the <u>300 eV </u>impact energy

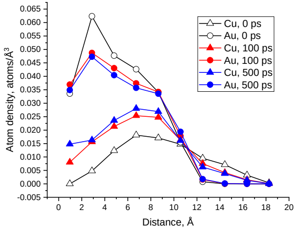
Ni-Al, Ar_1



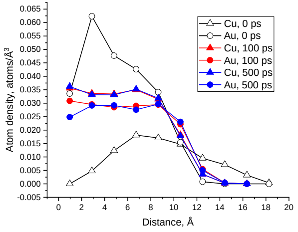
Ni-Al, Ar_{13}

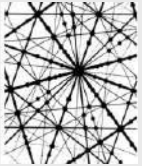


Cu-Au, Ar_1

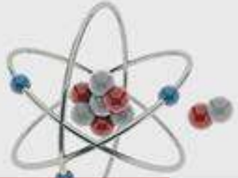


Cu-Au, Ar_{13}

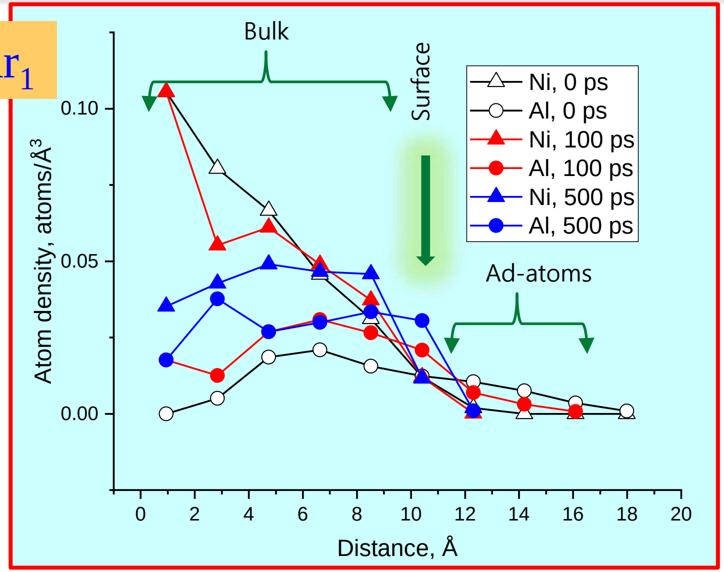




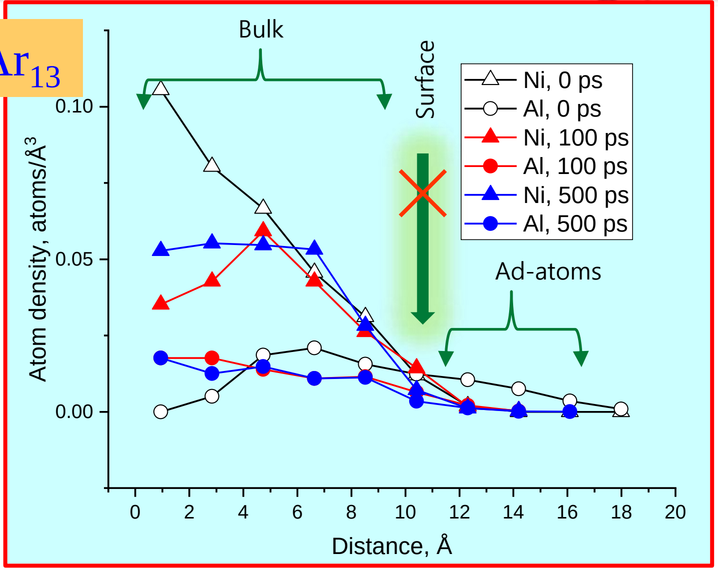
Spherical distributions of atomic densities of the mono-component parts in the clusters at the 1000 eV impact energy



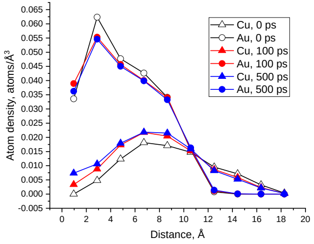
Ni-Al, Ar_1



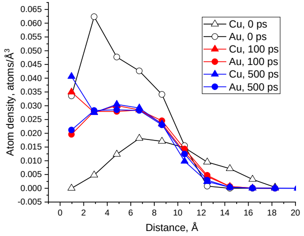
Ni-Al, Ar_{13}



Cu-Au, Ar_1



Cu-Au, Ar_{13}



Epilogue : conclusion and outlook

- ✓ The 100-500 ps evolution of the Ni-Al Janus-like cluster under up to 1.0 keV Ar_1 and Ar_{13} impacts was simulated and compared with the results for the Cu-Au and Cu-Bi clusters.

- ✓ The core-shell structure with predominantly Ni atoms in the inner part and Al atoms in the outer layer of the Ni-Al cluster was found at Ar single atom impact.

- ✓ An analogous mass transfer trend in the Ni-Al cluster was found at Ar_{13} cluster impacts, but the strong masking effect (excluding <100 eV impacts) of Al preferential sputtering, including noticeable thermal yield at extra high temperatures, does not allow a core-shell structure with predominantly Al atoms on the cluster surface to appear.

- ✓ After exposition of the Janus-like Cu-Bi clusters to Ar13 projectile with 300 eV and higher energy, Cu-enriched core and Bi-enriched shell were formed, while only partial coating with eccentricity of the atomic distributions took place at Ar1 impacts. The Cu-Au clusters undergo similar evolutions, and the correlation of the syntheses' intensities at Ar1 and Ar13 impacts also takes place.

- ✓ Tuning the energy and size of the bombarding particle is a promising tool of making bimetal clusters with desired space component distributions, but conditions of bombardment may vary.

Acknowledgements

The research is carried out using the equipment of the shared research facilities of

✓HPC computing resources at Lomonosov Moscow State University;

✓Sheared-Use Equipment Center of FSBI TISNCM, Troitsk, Moscow.

Thank you for your time!