Supplementary materials Molecular dynamics simulation of formation of Cu-Pt nanocontacts in the mechanically controlled break junction experiments

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1 Preparation of the initial Cu-Pt wire

Figure S1. Scheme of preparation of the initial Cu-Pt wire.

In order to prepare the initial Cu-Pt wire the following procedure is used (see Fig. S1):

- 1. Three-dimensional fcc lattice with Cu atoms is created. Periodic boundary conditions are applied to all three directions. Atoms in the cylinder in the center of the cell are considered as atoms from a wire.
- 2. Some of the Cu atoms inside the wire are randomly replaced with Pt atoms. Number of the replaced atoms is calculated according to the concentration of the Pt atoms.
- 3. The equilibrium Monte Carlo (MC) method [1] is used to rearrange atoms inside the wire. At the beginning of each MC step one Cu and one Pt atoms are randomly selected. After that, these two atoms are interchanged with probability $\exp(-\Delta E/k_{\rm B}T)$ if $\Delta E > 0$, or 1 if $\Delta E \le 0$, where $\Delta E = E_{\rm f} E_{\rm i}$ is the difference between the potential energies of the initial and the final states, $k_{\rm B}$ is the Boltzmann constant, T is the temperature. The canonical distribution of the Pt atoms inside the wire is achieved after 10^6 MC steps.
- 4. The wire is removed from the Cu bulk.
- 5. The wire is relaxed by means of the Molecular Statics (MS) method at zero temperature during 10⁴ MS steps.
- 6. The wire is thermalized by means of the Molecular Dynamics (MD) method at the temperature T. A chain of five Nosé-Hoover thermostats is employed to simulate the canonical ensemble [2–4]. The canonical distribution is achieved after 10^6 MD steps.

2 Stability of the structures

To check the stability of the structures from article [5] and from our simulation (Model 2 and Model 3) we made the following test. At the beginning, we put structures between copper electrodes consisting of 6 layers (2 bottom layers of lower electrode and 2 top layers of upper electrodes were fixed) with [111] orientation and made structure relaxation. We found that structures DZZ2 and DZZ4 (designations from the article [5]) are not stable after structure relaxation. The other structures are shown in Fig. S2.



Figure S2. Side view on the breaking area structures stable after structure relaxation. Brown balls symbolize Cu atoms and gray balls symbolize Pt atoms.

After that, we made several tests with structures presented in Fig. S2. Results of the tests are assembled in Table S1. Firstly, we found the boundaries of elastic deformations corresponding to compression $(-\Delta l)$ and elongation $(+\Delta l)$. Deformation of the structures DZZ1 and DZZ3 is ductile when strain is higher than 0.01 Å. The linear structure,

Model 2 and Model 3 are stable under deformations. Secondly, we heated the structures until their deformation was elastic. The structures DZZ1 and DZZ3 are stable only at 0 K. The linear structure is stable at temperatures lower than 50 K. The Models 2 and 3 are stable at temperatures lower than $\sim 350 - 400$ K. We would also like to note that the inelastic deformation of the linear structure leads to its destruction, while the inelastic deformation of the Model 2 and Model 3 leads to a ductile deformation.

	$_{ m linear}$	DZZ1	DZZ3	Model 2	Model 3
$-\Delta l, \text{ Å}$	1.6	0	0	1.4	3.6
$+\Delta l, \text{ Å}$	0.7	0	0	1.1	1.9
$\mathbf{T}, \ \mathbf{K}$	50	0	0	350	390

Table S1. Stability region boundaries of the breaking area structures that are stable after structure relaxation.

3 Orientation of the breaking area

Orientation of the breaking area of the nanocontact does not exactly coincide with the elongation direction. The following procedure was applied to find orientations of the breaking areas of the nanocontacts. Let us consider a spherical coordinate system in which the angle θ is measured from the elongation direction. Let us calculate S – sum of the distances between atoms from the breaking area and a random axis which orientation is given by angles θ and ϕ . If $\{\theta_{br}, \phi_{br}\} = \operatorname{argmin} S(\theta, \phi)$ then the angle between the orientation of the breaking area and the elongation direction is equal to θ_{br} . The average values of the θ_{br} are equal to zero. Root-mean-squared deviations of the θ_{br} (θ_{br}^{RMSD}) for all of the elongation directions ([100], [110] and [111]), relative Pt concentrations and temperatures are presented in Table S2.

Pt concentration, $\%$	0	5	10				15	20
Temperature, K	300	300	4.2	77.4	200	300	300	300
[100]	19	17	41	33	35	29	27	30
[110]	30	24	44	53	36	32	31	33
[111]	23	26	39	37	28	24	22	25

Table S2. Root-mean-squared deviations of the angles (in degrees) between the elongation directions and the directions of the breaking areas of the nanocontacts.

Let us discuss the dependence of the θ_{br}^{RMSD} on the relative Pt concentration, elongation direction and temperature. The values of the θ_{br}^{RMSD} corresponding to the elongation direction [110] are higher than for the elongation directions [100] and [111] at almost all temperatures and relative Pt concentrations. We do not observe any strong dependence of the θ_{br}^{RMSD} on the relative Pt concentration. However, we find that the values of the θ_{br}^{RMSD} corresponding to the elongation direction [100] and relative Pt concentration of less than 10 % are lower than the other values. Values of the θ_{br}^{RMSD} at high temperatures are lower than at low temperatures, because at low temperatures the breaking areas of the nanocontacts are very short (see Fig. 2 of the article) and their shape is more like a sphere than a cylinder. In the main text of the article we present a value of the θ_{br}^{RMSD} averaged over all of the elongation directions, relative Pt concentrations and temperatures. It is equal to 32°.

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