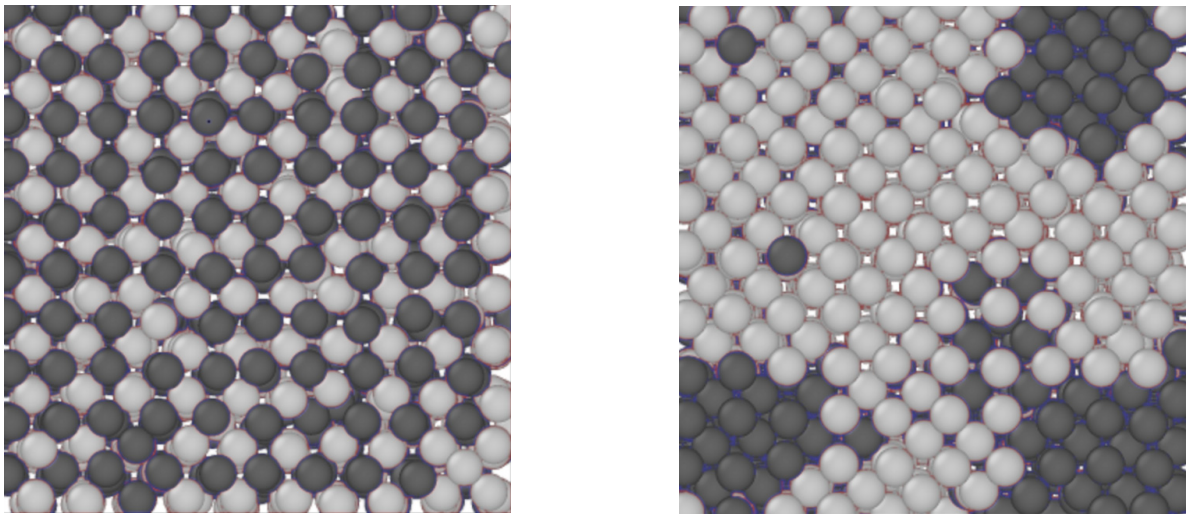
Supplementary material



a b

Fig. S1. Image of the atomic structure corresponding to the final stage of modeling the state of the system: WTa (a), WCr (b). Light marks the positions of tungsten atoms, dark — Ta and Cr.

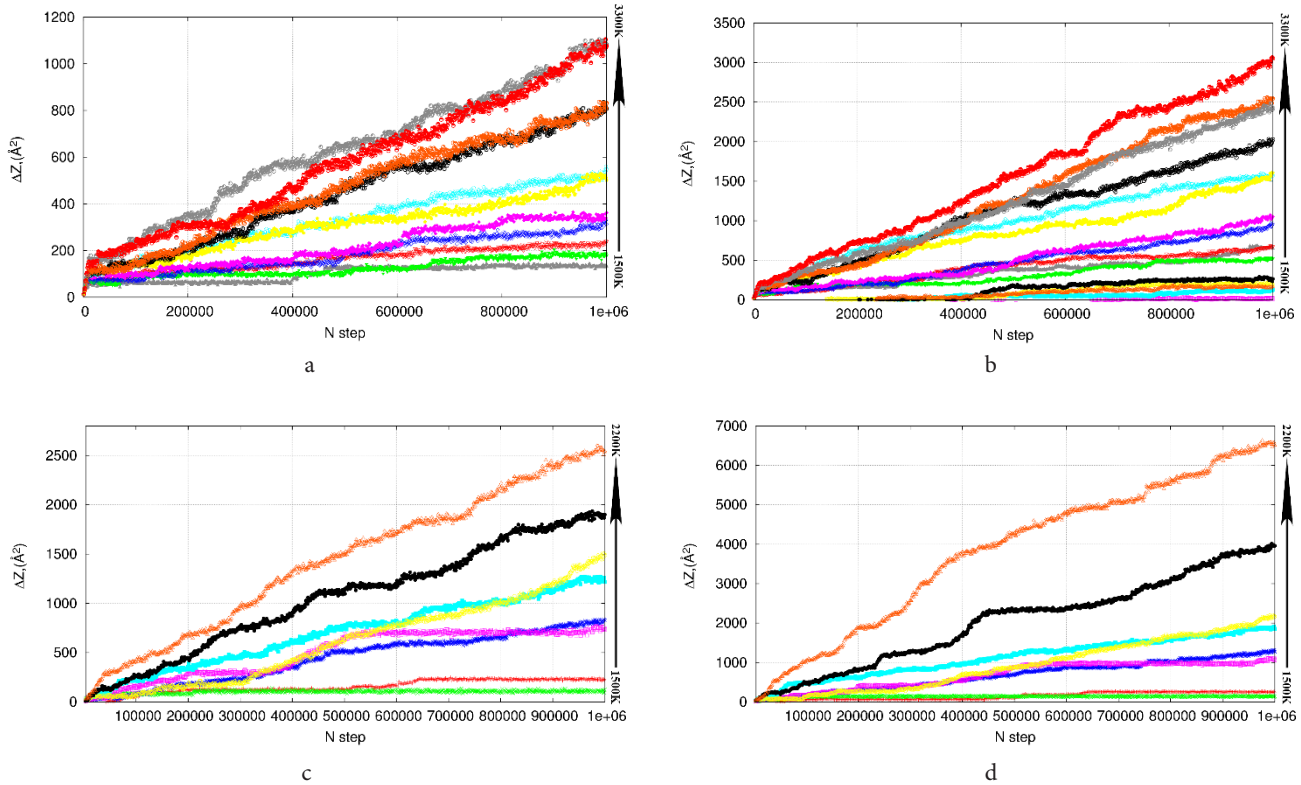


Fig. S2. (Color online) Sum of the squares of the atomic shifts in the thermodynamically nonequilibrium systems WTa (a, b) for the temperature range 1500 – 3300 Kand WCr (c, d) for the temperature range 1500 – 2200 K. Sum of squares of displacements of tungsten (a, c) and tantalum (b) atoms and chromium (d). On the *x*-axis, one step is equal to 2 fs. As the temperature increases, the slope of the dependence $\Delta Z(t)$ increases.

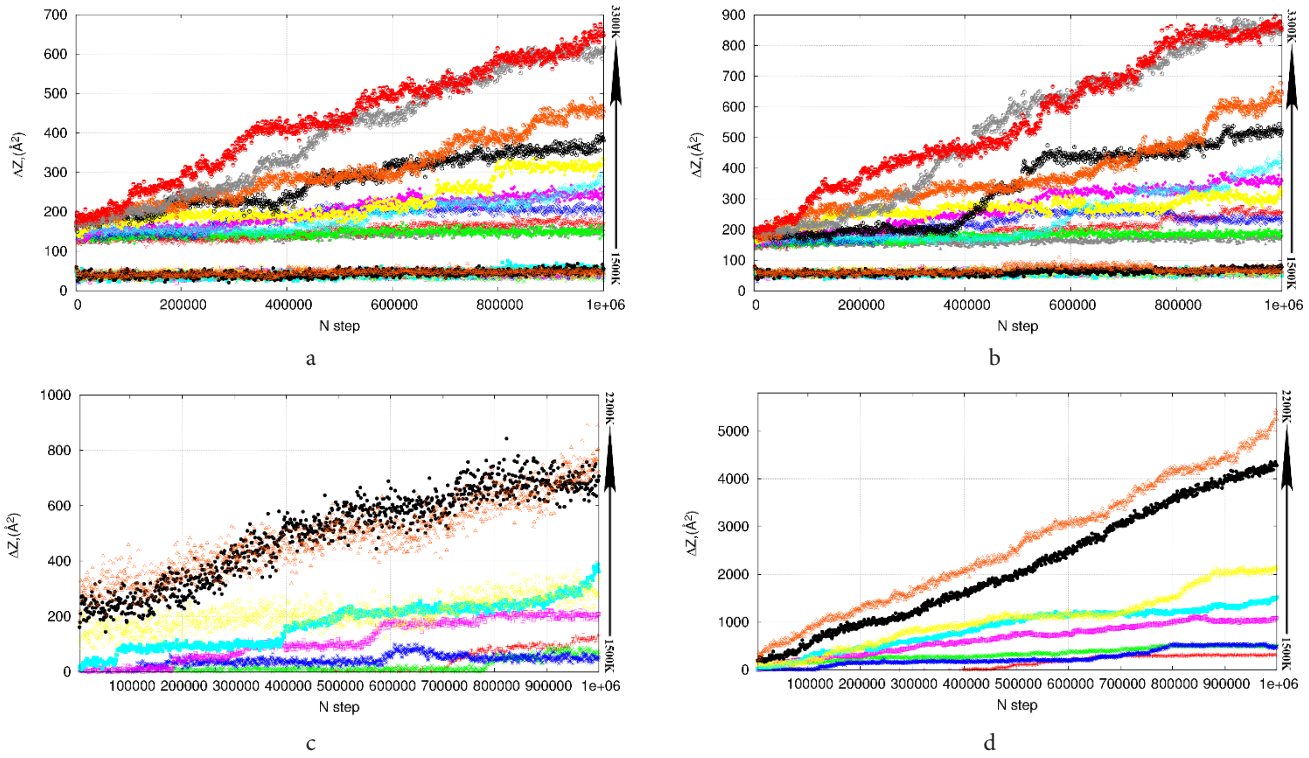


Fig. S3. (Color online) Dependence of the values of the sum of squares of the atomic shifts in thermodynamically equilibrium systems WTa (a, b) for the temperature range 1500 – 3300 K and WCr (c, d) for the temperature range 1500 – 2200 K. Sum of the squares of the displacements of tungsten (a, c) and tantalum (b) atoms and chromium (d). On the *x*-axis, one step corresponds to 2 fs. As the temperature increases, the slope of the dependence $\Delta Z(t)$ increases.

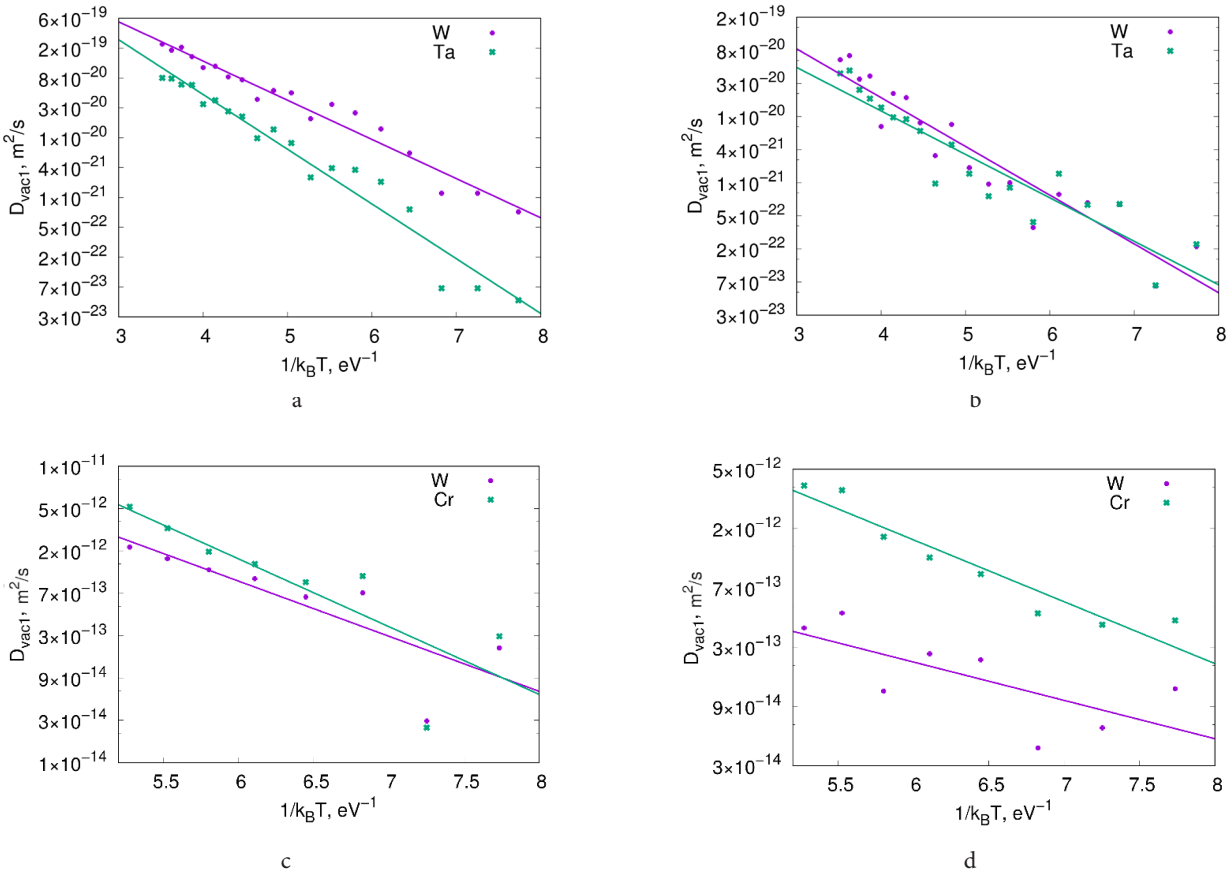


Fig. S4. (Color online) Interpolation by linear dependence of the logarithm of the calculated diffusion coefficients at the studied temperatures from $(1/kT)$. WTa system: in initial state (a), in equilibrium (b); WCr system: in initial state (c), in equilibrium (d).