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DEPARTMENT OF PHYSICS

MOLECULAR DYNAMICS SIMULATION OF THE DIFFUSION BEHAVIOUR IN Ti-Ag

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INTRODUCTION

Ti-Ag alloy system is interesting for its biocompatibility and bioadhesion properties, therefore it is promising for the production of bone implants. Classical molecular dynamics was used to simulate diffusion in the Ti-Ag system. It is very suitable for this purpose. It provides the positions of the atoms at each time step, from which it is possible to obtain the mean square displacement, which can be used to easily calculate the diffusion coefficient. The disadvantage, however, is the huge computational complexity and so we have to limit ourselves to a very small number of atoms (in this work only about 100,000) and very short time intervals (in this case only 6 ns).

MODEL SYSTEM

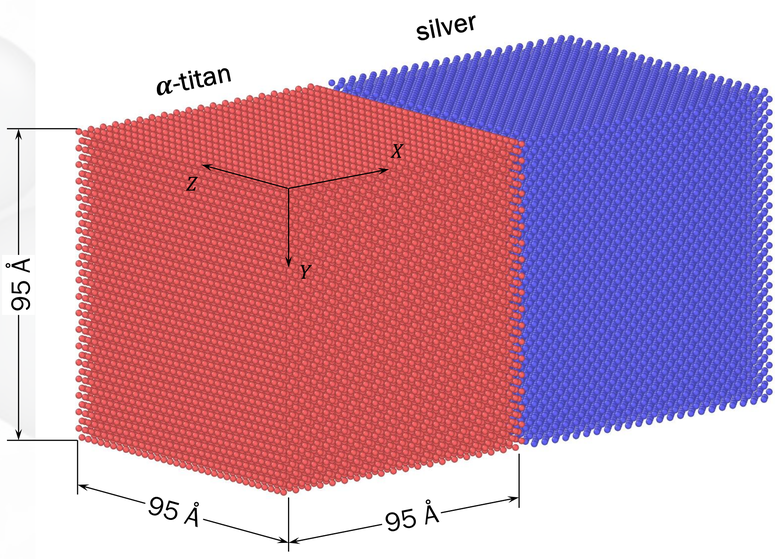

Fig. 1. *Initial configuration of the simulation. The red spheres represent titanium atoms arranged in a hcp structure and the blue spheres represent silver atoms arranged in a fcc structure.*

Simulations were performed using the LAMMPS with this setup:

- ✓ Diffusion model consisting of two bulks: one bulk was composed of titanium atoms arranged in a hcp (α-titanium) structure and the other was composed of silver atoms arranged in a fcc structure (Fig. 1).
- ✓ Simulation settings: 2NN-MEAM potential, NPT statistical ensemble, time step 0.002 ps, pressure 1 bar, Nosé-Hoover thermostat and barostat, periodic boundary conditions.
- ✓ The simulations were performed at 4 temperatures (850, 900, 950, 1000 K) for 6 ns (the visualization after 6 ns at 900 K is shown in Fig. 2).
- ✓ The diffusion coefficient was calculated for Ag in the [001] α-Ti direction and Ti in the [100] Ag direction using the mean square displacement (MSD) recorded during the simulation.
- ✓ The diffusion coefficient was estimated by the fitting of the linear region from the MSD and time curves (region 2 – 6 ns).

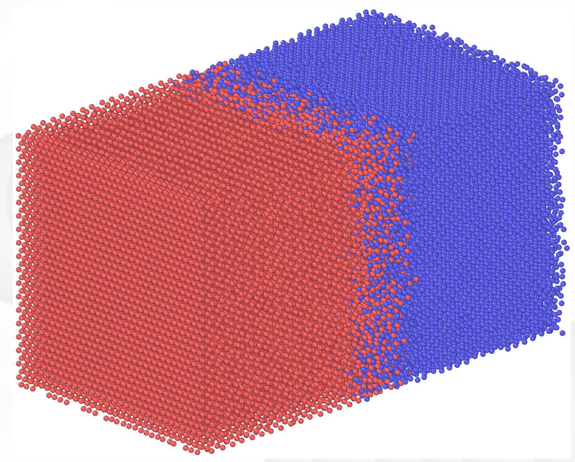

Fig. 2. *System after 6 ns of simulation at 900 K.*

RESULTS

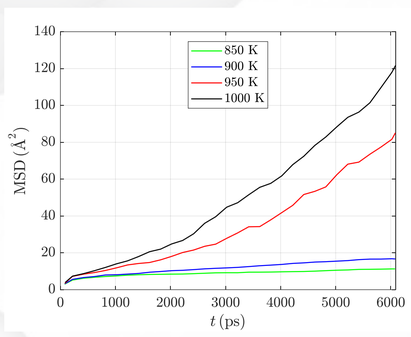

Fig. 3. *Time dependence of MSD for titanium atoms in silver at temperatures of 850, 900, 950 and 1000 K.*

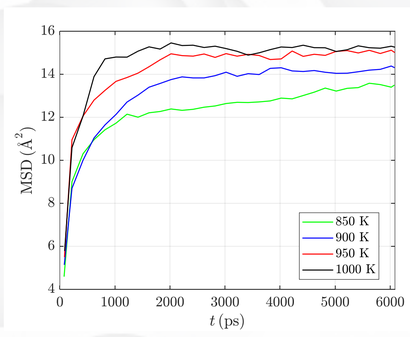

Fig. 4. *Time dependence of MSD for silver atoms in α-titanium at temperatures of 850, 900, 950 and 1000 K.*

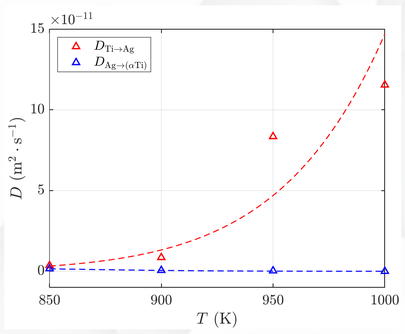

Fig. 5. *Dependence of the diffusion coefficient on the temperature of titanium in silver (red) and silver in α-titanium (blue).*

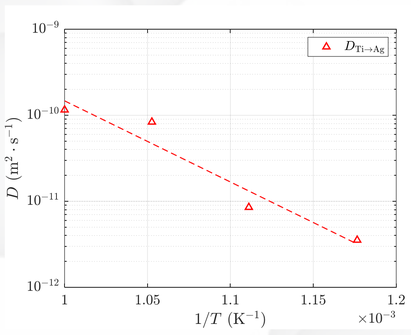

Fig. 6. *Dependence of the diffusion coefficient of titanium in silver on the inverse of the temperature.*

The MSD vs. time dependencies of titanium in the silver structure at 850, 900, 950 and 1000 K are shown in Fig. 3 and similarly the MSD of silver in α-titanium are shown in Fig. 4. After about 2 ns the MSD is stabilized. In the intervals of 2 - 6 ns, from which the diffusion coefficients are also evaluated, the completely different behaviour of titanium and silver can be seen. While the MSD of titanium in silver increases almost linearly, the MSD of silver in α-titanium is practically constant. This indicates that while titanium diffuses into silver, silver does not diffuse into α-titanium.

From the linear MSD regions (2 – 6 ns), the diffusion coefficient was fit as an Arrhenius equation

$$D = D_0 \exp\left(-\frac{E}{RT}\right).$$

Fig. 5 shows the calculated diffusion coefficients of titanium in silver ($D_{\mathrm{Ti}\to\mathrm{Ag}}$) and silver in α-titanium ($D_{\mathrm{Ag}\to(\alpha\mathrm{Ti})}$), and Fig. 6 shows the diffusion coefficient of titanium in silver as a linear dependence on the inverse of temperature. From the Arrhenius equation, the activation energy E of titanium was evaluated as $180.5\ \mathrm{kJ\cdot mol^{-1}}$ and the frequency of attempts D_0 as $0.4\ \mathrm{m^2\cdot s^{-1}}$. Because the diffusion coefficient of silver was practically constant (independent of temperature), it could not be evaluated as an Arrhenius equation and plotted in Fig. 6. It was not possible to evaluate its activation energy and frequency of attempts. Finally, concentration profiles were plotted at two times of 0.5 and 6 ns (Fig. 7).

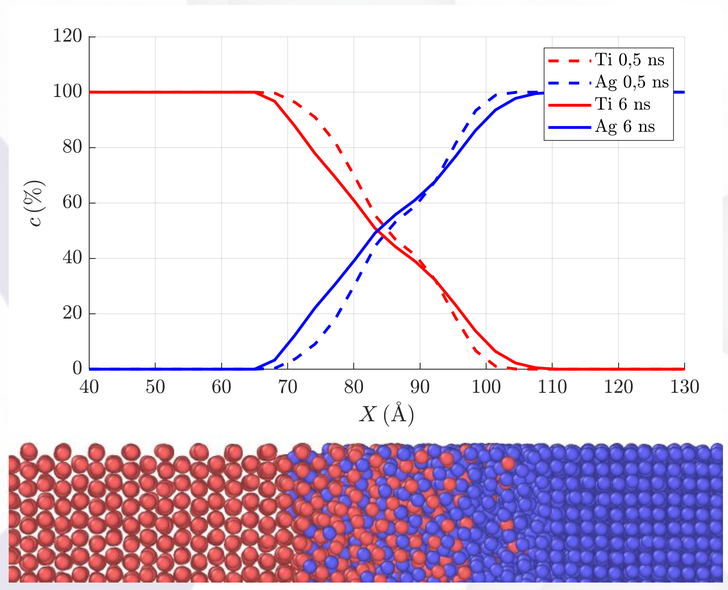

Fig. 7. *Concentration profiles of alpha titanium and silver at 0.5 ns and 6 ns. The visualization of the system below the graph is at 6 ns time.*

CONCLUSION

From the simulations, the dependence of the diffusion coefficient of titanium in the crystallographic direction [100] of silver in the temperature range 850 - 1000 K was found to be

$$D_{\mathrm{Ti}\to\mathrm{Ag}} = 0.4\ \cdot \exp\left(-\frac{180.5\ \mathrm{kJ\cdot mol^{-1}}}{RT}\right)\ \mathrm{m^2\cdot s^{-1}}\ .$$

The diffusion coefficient of silver in the crystallographic direction [001] of α-titanium was studied in the same way, but because it was constant with temperature, it could not be evaluated as an Arrhenius dependence and calculate the activation energy and frequency of attempts. Since the hcp structure of α-titanium exhibits a pronounced anisotropy of physical properties, it is possible that silver will diffuse in crystallographic directions other than [001]. This will be the focus of future research.

REFERENCES:

[1] Thompson, A. P. et al., LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Comp. Phys. Comm.*, 271:108171.

[2] Syarif, J. et al., Atomistic simulation of the diffusion behavior in Al-Fe. *Nuclear Materials and Energy*, 29:101073.

ACKNOWLEDGEMENT:

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