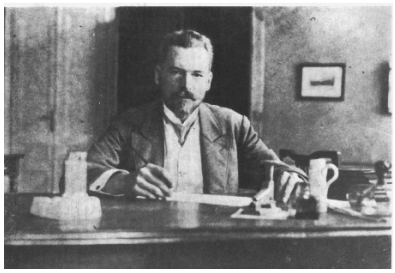

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Diffusion of nickel atoms into silver regimes in layered nanostructures- molecular dynamics simulations.

Monday, 27 September 2021 17:50 (5 minutes)

Silver and nickel composites are peculiar for many reasons. As pure, both of these metals exhibit fcc crystal structures, but their lattice constants are much different. Because in the solid state they are almost insoluble, in the case of flat surfaces it may result in occurring of superlattice arrangement resulting from the mistmatch of lattice constants, with silver atoms well separated from nickel atoms. When temperature is raised the situation changes. If only one silver nanolayer deposited on the nickel layer is heated, it disappears through the desorption mechanism. However, if a silver nanolayer is confined between two nickel layers, desorption mechanism is no longer possible. Now, since melting temperatures of nickel and silver are also very different, an interesting case to study occurs, when one nanolayer is solid and the other is liquid. Taking also into account that nanoparticles are already known to exhibit lowered temperature of melting, one expects that this phenomenon will occur also in the case of nanolayers. In the presentation we will show the results obtained from the molecular dynamics where a multilayered silver-nickel structure undergoes heating and cooling. Especially interesting result has been obtained for a structure that was very slowly cooled down from a completely liquid state. One observes here nickel atoms diffusing into silver regime and creation of the alloy nanolayer in coexistence at the same time with pure nickel layers. Such an effect – possibility to change silver nanolayer onto silver-nickel alloy nanolayer upon confinement at increased temperature has not been previously discussed. Other observed tendencies are also presented.

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