Whether quenched metal films should be amorphous or crystalline: molecular dynamics study

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In 50s A.P. Kobeko proposed a criterion which makes it possible to distinguish between solid, liquid and amorphous states of matter. According to this criterion, the radial distribution function (RDF) of a single crystal has several well resolved maxima, RDF of an amorphous body has only one well resolved maximum, and RDF of liquid has one poorly resolved maximum. And it is of interest that according to accurate electronographic data by S.I. Popel, such form of RDF typical for the amorphous state was really found for metal films obtained by means of the subsequent quenching and annealing processes. To study the structure of quenched metal islands films, we have used molecular dynamics (MD) method: our own computer program (involving the tight-binding potential) and the well-known open program LAMMPS (involving the embedded atom method). Then, two types of the solid substrate have been engaged in our MD experiments: Ni(100) and Si (100) faces. In computer experiments the quenched and relaxed single component island films were obtained by means of the nanodroplet spreading and by means of the molecular beam epitaxy. A comparative study of Ag and Au films formation was carried out under the same deposition conditions on Ni (100) face at 300K with the following quenching at a high cooling rate (10^{10} K/s) down to the helium temperature (4K). Such a quenching rate and so low final temperature are used in direct experiments to obtain amorphous metal films using the vapor condensation on the cooled substrate. It has been found that even at so high cooling rates, the Ag beam condensation results in the 2D single crystal formation (see Fig. 1a). At the same time, the RDF for Au films shown in Fig. 1b seems to look like an amorphous type. However, a more detailed analysis results in a conclusion that the Au films under consideration should be rather interpreted as 2D-polycristals.

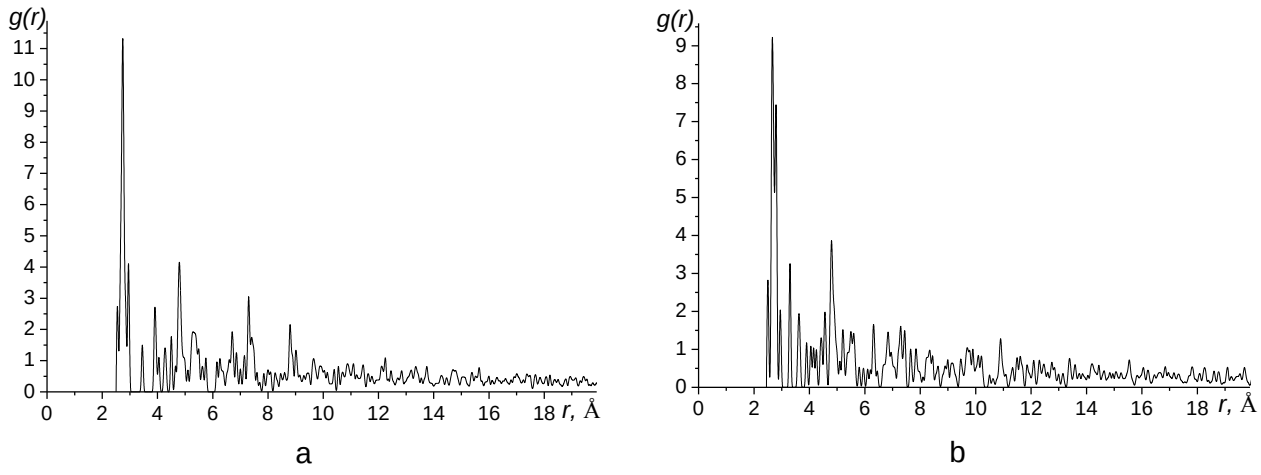

Fig.1. RDF for the Ag (a) and Au (b) films on Ni (100) face, respectively

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