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Secondary emission of neutral and charged particles from intermetallic single-crystal

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ABSTRACT

Sputtering, secondary ion and secondary electron emission were studied experimentally for an intermetallic Ni_4Mo compound with high corrosion resistance and great hardness, which is used as material for constructing components of rockets and nuclear reactors. The process of sputtering was analyzed by molecular dynamics simulations of Ni_4Mo (111) face for unchanged and changed composition (with segregation) of topmost layers of a disordered and ordered crystal. Predominant exit of Ni and Mo atoms in close-packed directions was observed and explained by correlated collisions. Both nickel and molybdenum atoms are ejected in the same crystallographic directions for a disordered crystal. For an ordered crystal the nickel atoms deviate from these directions. The origin of sputtering and number of ejected particles generated has been calculated. For secondary electron emission from the (111) Ni_4Mo face the maxima in close-packed directions were obtained experimentally and explained by scattering of primary and secondary electrons on atoms located in the lateral sides of open channels.

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1. Introduction

Research on neutral and charged particle emission under ion bombardment of Ni_4Mo single-crystals is important for understanding the mechanisms of particle interaction with a surface of intermetallic compound and for practical applications, e.g. in secondary ion mass spectrometry, catalysis, and in production of hard refractory coatings [1].

Intermetallic compounds with a significant difference of component masses, such as Ni_4Mo, are characterized by the difference between the surface and bulk structures, compositions, and properties [1–4]. Among them are such properties as surface segregation, surface ordering, and reconstruction [5]. The processes of ordering in such crystals were studied experimentally [6–9] and by numerical simulation [5,9]. In general, these compounds are thermally treated to obtain an ordered structure [6,7]. The intermetallic crystals can be also ordered using electron [6,7], neutron [7], and ion irradiation [8,9]. In these cases, as shown in Ref. [9], radiation-enhanced ordering is not associated with additional heating during irradiation.

It was shown that the segregation leads to a change of surface composition of the three top layers of intermetallic compounds, which is different for different faces of crystals. For instance, the top layer of the (001) NiPd face contains 80% of Pd, whereas the second layer has no Pd and the third layer has 64% of Pd [5]. Such changes in composition of surface layers are caused by the interplay of two competing factors: the mechanical stress (that leads to the segregation of the heavy component of the compound on a surface) and the various chemical interactions (that result in short-scale ordering) [5–7].

The sputtering and secondary ion emission from Ni_4Mo single-crystal was first studied in Ref. [10] for ion irradiation of the (001) face. The preferential yield of nickel (light component) was observed which is facilitated by the lower binding energy of Ni in comparison with Mo. Different angular distributions of emitted secondary ions for ordered and disordered (i.e. for randomly placed of Ni and Mo atoms) single-crystals were obtained. However, the experimental setup in Ref. [10] did not allow independent variations of observation angles for primary and secondary ions. In the present work, we eliminated this disadvantage, so that correct studies of azimuthal and polar angle distributions of secondary Ni and Mo ions from the Ni_4Mo single-crystal could be made.

The process of sputtering was studied also by molecular dynamics simulations. Polar and azimuthal angular distribution of sputtering under irradiation Ni_4Mo (111) face by 10 keV Ar^+ ions at normal incidence ($\alpha = 0°$) for unchanged and changed composition

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(i.e. with segregation of topmost surface layers of disordered and ordered crystal) were analyzed.

2. MD simulation

Simulation of sputtering was performed for the (111) face of ordered and disordered Ni_4Mo single-crystal with tetragonal lattice.

The crystalline structure of ordered Ni_4Mo single-crystal is illustrated in Fig. 1.

The sputtering of Ni_4Mo crystals was calculated using the molecular dynamics model with a moving single-crystal block of atoms [11–13]. At fixed moments in time, the interaction of a moving (active) particle with target atoms was considered. The nearest atoms form a block whose radius is equal to the radius of the fifth coordination sphere. In the resulting structure, an incident ion and target atoms can move and interact with each other. When an active particle moved, the block moved too and formed the sphere around the particle. If the energy acquired by interacting target atoms was higher than the threshold level (equal to the binding energy), the positions and momenta of these atoms were recorded and, subsequently, their further motion was calculated.

The block of atoms had no time to exhibit instability, because the sputtering of an atom is a short-time process (its duration is approximately 10^{-13} s [14] from the moment of impact of ion). This model made it possible to trace the particle trajectory at large (hundreds of angstroms) distances from the place of the ion incidence.

The equations of motion were integrated using a modified Euler predictor-corrector scheme that is stable [14]. Inelastic losses were computed according to the Firsov formula [15]. Thermal oscillations of atoms were assumed to be uncorrelated.

Lattice distance a, c and binding energy E_b were chosen from experimental data: $a = 5.720$ Å, $c = 3.564$ Å and $E_b = 4.2$ eV [4]. The interaction potential was determined in the following form [16]: $U(r) = A_{bm}\cdot\exp(-r/a_{bm}) + (A_b/r)\cdot\exp(-2r/a_{bm})$, where $A_{bm} = 52(Z_1Z_2)^{3/4}$, $a_{bm} = 0.219$ Å, $A_b = k(Z_1Z_2e^2)$, Z_1 and Z_2 – are the atomic numbers of the ion and target atom, respectively; r is the vector radius; and k is an adjustable parameter of the order of unity. In the computation, the following parameters were determined: the sputtered atom's momentum, the length of the sputtering cascade path, the sputtering time, the sputtered atom's generation number L, and the depth of the origin x_0 of sputtering.

3. Experiment

The patterns of sputtering the (111) Ni_4Mo face was obtained using the system shown schematically in Fig. 2.

The setup for sputtering contains the ion source of Ardenne [17], improved as discussed in Ref. [18], which allowed well-focused beams of argon ions with a current density of 1 mA/sm^2 at energy $E_0 = 10$ keV to be obtained. The ion beam, after acceleration and focusing by a single electrostatic lens, passed through a hole in a quartz screen and bombarded the sample on the area with diameter of 2 mm. The dose of irradiation was measured by current integrator. A glass collector for sputtered particles was placed parallel to the studied surface in front of the sample in the distance of 15 mm. Spot pattern of sputtered particles was used to determine the orientation of single-crystal samples.

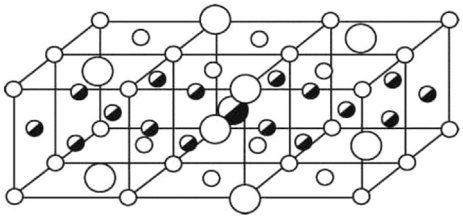

Fig. 1. A structure of ordered Ni_4Mo single-crystal with tetragonal lattice. Large and small circles correspond to Mo and Ni atoms, respectively. Semi-closed circles are atoms arranged within the lattice.

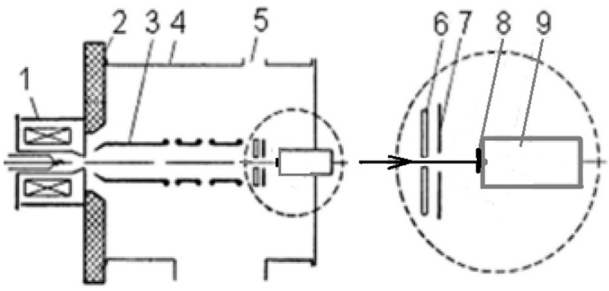

Fig. 2. Sputtering system. 1 – ion source, 2 – insulator, 3 – electrostatic lens, 4 – container, 5 – window, 6 – quartz screen, 7 and 10 – glass collectors, 8 – specimen, 9 – holder.

For studying the secondary ion emission it is important to simultaneously determine the angular and energy distributions of mass-separated secondary species. In our work, these measurements have been performed by a specially designed and constructed setup with a mobile 180° spherical energy analyzer linked to an immobile quadrupole mass spectrometer as shown in Fig. 3.

The secondary ion flux was focused in two directions, which ensured a high transmission coefficient and allowed axis-symmetric optics to be used. The energy resolution was about 0.5 eV (at transmission energy of 20 eV) and the ion mass range was 1–350 amu. The sample chamber was evacuated by a magnetic discharge pump to a residual pressure on the order of 10^{-9} mbar.

The primary ions were incident on the target at an angle $\alpha = 0°$ relative to the normal to the surface. The polar angle θ of observation of the secondary ion emission could be varied within 90° by rotating the energy analyzer. The yield of secondary ions I^+ was determined either by integrating the mass peak at the certain ion energy or by integrating the energy spectra of ions.

The secondary electron emission was measured by the scanning electron microscope (LEO 14XX (VP)). We use a passing of 1 nA current through a crystal. Some times we measured also back-scattered and secondary electrons using a Faraday cup. The energies of primary electrons were 10 keV.

The topography of surface has been studied by the scanning electron microscope (LEO-1455 (Carl Zeiss)) and by the atomic force

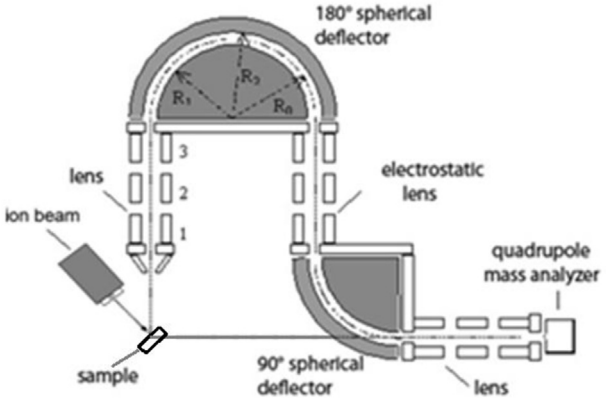

Fig. 3. Schematic diagram of experimental arrangement.

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