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Concentration and temperature dependence of short-range order in Ni–Ta solid solutions using the X-ray diffraction method.

By FARID A. KHWAJA,* *International Centre for Theoretical Physics, Trieste, Italy* and ANIS ALAM, *Department of Physics, Punjab University, New Campus, Lahore, Pakistan*

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Abstract

Diffuse X-ray scattering investigations on the existence of short-range order (SRO) have been carried out in the Ni–Ta system for different concentrations and annealing temperatures. The values of the SRO parameters for the first coordination shell are observed to have anomalously large negative values for all the samples studied. These values of α_1 depend upon the annealing temperatures and the concentration of Ta atoms in the Ni–Ta system. The results of the theoretical predictions of the ordering potential, obtained with the formulae of the electronic theory of SRO, confirm the existence of very strong attractive correlation between the atoms of the different species in this system.

The possibility of the existence of local order in Ni-rich alloys of Ni–Nb and Ni–Ta was discussed in a series of papers (Baer, 1966; Chessin, Arajs & Colvin, 1964; Alizade & Magarrov, 1968; Larson, Taggart & Polonis, 1970; Vander Wekken, Taggart & Polonis, 1971) using an indirect method. The anomalous behaviour of electrical resistivity, paramagnetic susceptibility and thermomagnetic properties were explained as being due to the existence of short-range order (SRO) in the form of local order in these systems. It is pointed out that the influence of the concentration of Nb and Ta on the behaviour of the physical properties of ferromagnetic nickel is identical. The direct determination of the existence of SRO in Ni–10 at.% Ta has also been reported (McManus, 1965).

The diffuse X-ray scattering measurements were carried out in three polycrystalline samples consisting of 3, 7 and 11 at.% Ta in Ni on a diffractometer Dron-1 using line-focused Co and Cu $K\alpha$ radiation, monochromated by reflections from a single crystal of Si [reflection plane (111)]. The heat treatments of the samples from 270 to 1520 K were performed in an atmosphere of purified argon and the annealed samples were quenched rapidly in diffusion oil. The SRO and size-effect (linear and quadratic) dependent diffuse X-ray scattering intensity was determined by subtracting the parasitic terms from the measured intensity and subsequently put upon an absolute scale (electron units per atom).

The diffuse X-ray intensity data is shown in Fig. 1 as a function of scattering angle θ in the region near the first two superstructural lines for three concentrations in the Ni–Ta system. Curve 3 corresponds to the intensity from a plastically deformed sample of Ni–11 at.% Ta and curves 2 and 1 correspond to diffuse intensity from samples annealed at 1470 K of Ni–7 at.% Ta and Na–3 at.% Ta respectively. The appearance of sharp maxima in the region of angles close to the superstructural positions {100} and {110} is the evidence for the existence of SRO in these alloys. A decrease in diffuse intensity may also be seen in Fig. 1 as the Ta concentration in the Ni–Ta system decreases.

The values of the SRO and size-effect parameters ($\alpha_{i=1,2,\ldots}$ and a_g) calculated from the measured diffused scattering intensity from these samples using the relationship given by Iveronova & Katsnelson (1977) are given in Table 1. It is seen that the values of the SRO parameters for the first coordination sphere α_1 are negative and their absolute values are greater than the limiting values $\alpha_{1\,\mathrm{lim}} = |-C_A/C_B| = |1 - P_{AB}/C_B|$ for all the cases under consideration. On the other hand, the values of α_2 are equivalent to their limiting values. Analogous values of α_1 were also found for Cu–16 at.% Al (Iveronova, Katsnelson & Revkevich, 1966; Houska & Averbach, 1959; Kagan, Somekov & Umanskiy, 1959), for Ni–6·3 at.% Al (Katsnelson & Dazhaev, 1970), for Cu–29·2 at.% Pt (Iveronova, Katsnelson, Kondrateva & Revkevich, 1973), for Ni–13 at.% W (Katsnelson, Alimov, Dazhaev & Silonov, 1968) and for Al–10 at.% Ag (Lashko, 1962). The peculiar

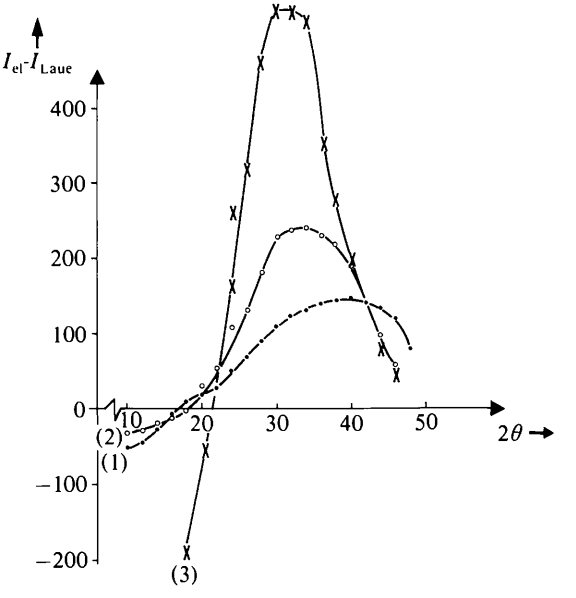

Fig. 1. The dependence of $I_{el} - I_{Laue}$ as a function of scattering angle 2θ for the three concentrations studied of the Ni–Ta system. —●— Ni–3 at.% Ta alloy annealed at 1470 K and quenched in oil. —○— Ni–7 at.% Ta alloy annealed at 1470 K and quenched in oil. —×— Plastically deformed sample of Ni–10 at.% Ta alloy.

* Permanent address: Department of Physics, Quaid-i-Azam University, Islamabad, Pakistan.

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Table 1. *The values of the SRO parameters and linear and quadratic size effects for the* Ni–Ta *system*

	α_1	α_2	α_3	a_g	a_g^2
Ni–3 at.% Ta	−0·06	−0·08	−0·02	0·12	0·26
Ni–7 at.% Ta	−0·13	0·23	−0·02	0·19	0·52
Ni–11 at.% Ta	−0·16	0·18	−0·08	0·20	0·54

variation in the value of the SRO parameter α_1 as a function of temperature and time is explained in all these papers by the 'appearance in the alloy, at a certain stage of annealing, of a superfine structure', *i.e.* the so-called local order. The values of the SRO parameters given in Table 1 are the effective values averaged over the submicroregions of excess and impoverished concentration using the method given by Iveronova & Katsnelson (1965).

It is worth mentioning that a very large value of the quadratic size effect found for these alloys predict a strong static distortion existing in the lattices of the Ni–Ta system. However, it is still not possible to explain such a significant value of the size effect in this system. Apparently, the impoverished matrix of the solvent causes additional static distortion in the submicroregions. In our opinion the physical properties such as microhardness depending upon the static distortion in the lattice should be investigated in these alloys.

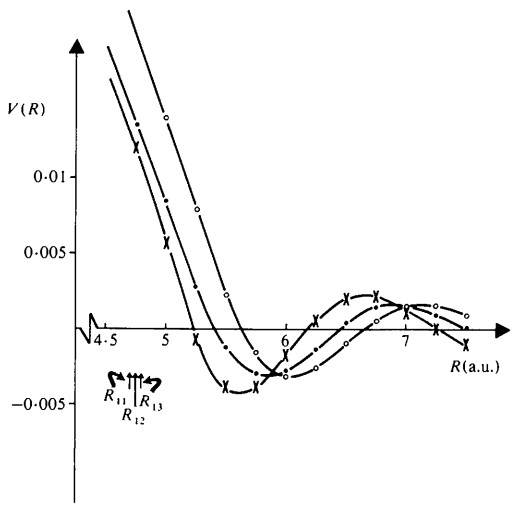

Fig. 2. The variation of ordering potential with the concentration of the Ta atoms in the Ni–Ta system as a function of the interatomic distance R. R_{11}, R_{12}, R_{13} denote the positions of the nearest neighbours for Ni–3, –7 and –10 at.% Ta, respectively. —×— Ni–3 at.% Ta; —●— Ni–7 at.% Ta; —○— Ni–10 at.% Ta.

In order to discuss theoretically the values of the SRO parameter for this system we have calculated the ordering potential with the relationship given by Khwaja, Katsnelson, Silonov & Khruschov (1977).

The results of the numerical calculation of the ordering potential $V(R)$ as a function of interatomic distance R are shown in Fig. 2 for Ni–3, –7 and –11 at.% Ta. The arrows R_{11}, R_{12}, and R_{13} represent the first nearest-neighbour distances for the three concentrations of the Ni–Ta system. It is seen that the values of the ordering potential for the first coordination shell are positive for all the three concentrations of the Ni–Ta system. Such a large positive value of the ordering potential for the first shell explains the presence of local order found experimentally in these alloys. From Fig. 2 one also observes the sharp dependence of the ordering potential upon the concentration of Ta atoms in the Ni–Ta system.

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