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Quasilocal vibrations produced in dilute $V_{1-x}Pt_x$ alloys under conditions of a strong restructuring of phonon spectrum of V

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Results are presented of the measurements of the spectra of inelastic incoherent scattering of neutrons by $V_{1-x}Pt_x$ alloys ($x = 5$ and 7 at.%). In the low-frequency regions of the spectra, quasilocal vibrations (QLV) are observed and are connected with introduction of the heavy impurity Pt atoms into the V. The energy position of the QLV is shifted in the region of higher values in comparison with those expected in isotopic-substitution model. Introduction of the Pt atoms leads also to a shift of the entire spectrum towards higher frequencies. The shift of the QLV and of the entire spectrum depends on the concentration of the impurity atoms. The energy position of the QLV can be satisfactorily explained within the framework of isotopic substitution using a renormalized spectrum of the original lattice.

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INTRODUCTION

Of great significance in the understanding of the physical properties of real crystals, is the investigation of alloys with sufficiently small contents of impurity atoms, when the impurity atoms can be regarded as isolated. In this case the theoretical interpretation of the experimental data becomes greatly simplified.

Even the first investigations of a number of dilute alloys, carried out both with the aid of the neutron-scattering method and by measuring the low-temperature heat capacity,^[1-3] have shown that in all cases new vibrational states are produced, due to the introduction of the impurity atoms. Depending on the value of the mass-difference parameter $\varepsilon = 1 - M_1/M_0$ (M_0 and M_1 are respectively the masses of the matrix and impurity atoms,) the introduction of impurity atoms leads to formation of either quasilocal vibrations (QLV) or local vibrations (LV). It turns out here that the energy position of the observed additional singularities in the spectra cannot be explained in most cases within the framework of the simplest model of isotopic substitution.

The introduction of a new parameter^[4] τ determined by means of a best fit of the experimental results to the calculation data yields information concerning a certain effective change of the local force constants.

However, in the study of alloys of non-isoelectronic elements one observes not only the formation of impurity states, but also a noticeable deformation of the entire spectrum of the initial lattice, which manifests itself in a shift of the spectrum towards higher energies. The deformation is larger the greater the difference between the electronic properties of the alloyed elements and the higher the concentration of the impurity atoms. Thus, introduction of the parameter τ , which takes into account the change of the local force constants, does not explain the influence of the deformation of the entire spectrum on the formation of the QLV.

From among the vanadium-base alloys investigated by us,^[5,6] the strongest restructuring of the initial spectrum should be expected for alloys with platinum impurity. In addition, in disordered solid solutions of V with Pt there is no noticeable change of the lattice

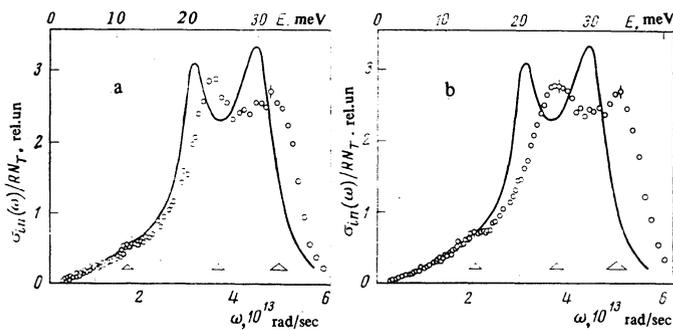


FIG. 1. Experimental functions $\sigma_m(\omega)/RN_T$: a— for the alloy $V_{0.95}Pt_{0.05}$, b— $V_{0.93}Pt_{0.07}$; solid curves—the function $g(\omega)$ for pure V.

parameter, so that the additional deformation of the phonon spectrum of V, due to the change of the volume of the unit cell following introduction of the impurity, is eliminated. The interest in these alloys was stimulated also by the fact that an investigation^[7] of the alloy $V_{0.95}Pt_{0.05}$ revealed no QLV, whereas it followed from^[5,6] that the QLV should manifest themselves quite distinctly at this ratio of the neutron masses and scattering amplitudes for the matrix and impurity atoms.

We have therefore investigated alloys of V with Pt impurity for the purpose of ascertaining the influence of of the restructuring of the phonon spectrum of the vanadium atoms on the formation of the QLV.

MEASUREMENTS. DISCUSSION OF RESULTS

The investigations were made on alloy samples of two compositions: $V_{0.95}Pt_{0.05}$ and $V_{0.93}Pt_{0.07}$. The samples were obtained by smelting vanadium of brand VEL-1 and platinum 99.7% pure in an arc furnace in an atmosphere of purified argon. Neutron-diffraction, x-ray diffraction, and metallographic analyses have shown that the samples are disordered solid solutions based on the bcc lattice of V. The lattice parameters of the alloys $V_{1-x}Pt_x$ do not differ, within $\pm 0.15\%$, from the lattice parameter of pure V.

The spectra of the neutrons elastically scattered by the $V_{1-x}Pt_x$ alloys were measured with a time-of-flight spectrometer and a source of cold neutrons.^[8] The samples were placed in a "transmission" position. The neutrons scattered by the sample were registered by four detectors placed at angles 90, 75, 60, and 45°. The measurements of each alloy sample lasted about 100 hours, thereby ensuring a statistical error of $\sim 4\%$ in the spectral region of interest, namely at low frequencies. The total energy resolution of the spectrometer in the interval of the resolved frequencies of the initial spectrum range from 10 to 6% and is indicated by the triangles in Fig. 1.

The spectra of neutrons inelastically scattered by disordered substitution-type solid solutions based on the bcc lattice of V, neglecting the small value of the amplitude of the coherent scattering by the V atoms, can be represented in the form

$$\sigma^{in}(\omega)/RN_T \approx a_0^2 K_{latt}(\omega) + c(a_1^2 - a_0^2) K_{imp}(\omega). \quad (1)$$

where $K_{latt}(\omega)$ and $K_{imp}(\omega)$ are the frequency Fourier components of the pair correlation functions constructed on the displacement operators of arbitrary atoms of the alloy and of the impurity, respectively; a_0 and a_1 are the total amplitudes for neutron scattering by the atoms of the matrix and the impurity; R is the energy of the recoil from an individual nucleus; $N_T = (e^{\omega/T} - 1)^{-1}$; c is the concentration of the impurity atoms.

The measurement results for both alloys are shown in Fig. 1. The ordinates represent the function $\sigma^{in}(\omega)/RN_T$, which goes over at zero concentration of the impurity atoms into the phonon spectrum of the initial lattice $g_0(\omega)$. For comparison, we show the function $g_0(\omega)$ obtained in^[5] for pure V. The low-frequency region of the "phonon" spectrum of each alloy reveals a singularity in the form of a maximum, the position of which shifts towards higher frequencies with increasing concentration of the Pt atom impurity. No such dependence was observed earlier in the energy position of the QLV. The appearance of a singularity in the low-frequency part of the "phonon" spectrum of the alloy, as seen from (1), is due to the positive ($a_1 > a_0$) contribution of the density of the vibrational states of the impurity atoms ($K_{imp}(\omega)$), which has a resonant character when the QLV appear. In addition, a shift of the main singularities of the entire spectrum of the V atoms into the region of higher energies is observed, although in the isotopic-substitution model the introduction of heavy impurity atoms should always lead to a softening of the initial spectrum. Within the limits of the experimental accuracy, the relative shift $\Delta\omega/\omega$ of the end-point frequency of the spectrum is proportional to the concentration of the Pt impurity atoms and amounts to 0.12 for the alloy $V_{0.95}Pt_{0.05}$ and 0.17 for the alloy $V_{0.93}Pt_{0.07}$.

In view of this character of the deformation of the initial spectrum of V, the previously employed description of the impurity systems within the framework of perturbation theory are no longer correct enough. A rigorous solution of the problem of the impurity state in this case calls for allowance for the influence of not only the mass difference but also the difference in the electronic properties of the components of the alloy causes the restructuring of the spectrum of the vibrational excitations of the initial matrix. It follows from the experimental data that the restructuring of the initial spectrum, due to the introduction of heavy impurity atoms, has a twofold character. On the one hand, owing to the mass difference of the matrix and impurity atoms, QLV are produced in a narrow interval of low frequencies. On the other hand, the difference between the electronic properties of the components of the alloy causes the phonon spectrum of the alloy to acquire already a new interval of allowed frequencies. It becomes therefore possible to analyze the deformation of the initial spectrum as a result of the mass difference within the framework of perturbation theory, by using as the zeroth approximation the spectrum of V renormalized to allow for the changes in the electronic subsystem.

Figure 2 shows the phonon spectrum of pure V and the renormalized V spectra following addition of 5 and 7 at. % Pt. The latter spectra are the smoothed-out-func-

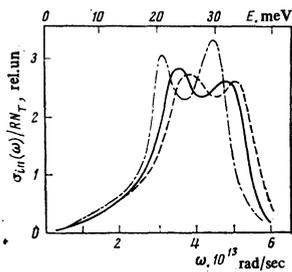


FIG. 2. Renormalized spectra: dash-dot curve—phonon spectrum of pure V; solid curve—“phonon” spectrum of V deformed by introduction of 5 at.% Pt; dashed curve—“phonon” spectrum of V deformed by introducing 7 at.% Pt.

tions reconstructed from the experimental data without the low-frequency singularities due to the presence of the heavy Pt atoms in the V. Starting out with these spectra, we calculated the density of the vibrational states of the impurity Pt atoms in the isotopic approximation and with account taken of the change of the local force constants of the interaction for different values of the parameter τ . Figure 3 shows the results of an experimental determination of the vibrations of the impurity atoms (a) and the results of the theoretical calculations (b). It is seen that as the renormalized spectrum becomes harder, the position of the QLV shifts towards higher frequencies. This shift is accompanied also by a smearing of the spectral distribution.

Thus, the introduction of heavy impurity Pt atoms into a vanadium matrix leads to the formation of QLV whose energy position shifts towards higher frequencies with increasing impurity-atom content. In addition, the addition of the non-isoelectronic platinum atoms to the vanadium leads also to a restructuring of the electronic subsystem and, as a consequence, causes a strong deformation of the dynamics of the initial lattice.

A comparison of the experimental and theoretical positions of the QLV shows that the best agreement for the renormalized spectrum is observed in the case of the isotopic approximation. This suggests that a certain effective interaction, which is the same for all the alloy components, is established in the alloy.

The energy position of the QLV is determined not by the initial phonon spectrum of the vanadium, but by the spectrum renormalized as the result of the changes in the electronic subsystem, and this renormalized spectrum depends in turn on the concrete composition of the alloy.

Such an appreciable restructuring of the phonon spectrum of V following introduction of Pt atoms is probably accompanied by substantial changes in the electron density on the Fermi surface, in the electron-phonon inter-

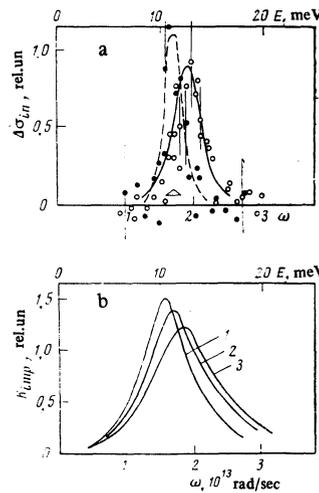


FIG. 3. Experimental (a) and theoretical (b) densities of the vibrations of Pt atoms: a) ●—in the alloy $V_{0.95}Pt_{0.05}$, ○—in the alloy $V_{0.93}Pt_{0.07}$; b) without a change of the force constants and using the spectrum of: 1—V, 2— $V_{0.95}Pt_{0.05}$, 3— $V_{0.93}Pt_{0.07}$.

action, and in the value of the superconducting transition temperature. It is therefore undoubtedly of interest to measure the low-temperature specific heat and the temperature dependence of the resistivity of the same alloys.

In conclusion, it is our pleasant duty to thank A. P. Zhernov for taking part in a discussion of the results, and V. G. Fedorov, Yu. V. Sereda, and A. M. Finogin with help with the measurements.

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