STUDIES OF ORIENTATION EFFECTS IN CRYSTALS BY ISOLATED RESONANCES IN NUCLEAR REACTIONS

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The isolated resonance of a nuclear reaction occurring at impurity interstitial atoms has been used for the first time to study orientation effects. The resonance of the $^{13}C(p,\gamma)^{14}N$ reaction, provided the proton energy of 1.7476 MeV, was used to investigate the proton flux distribution in the (0001) planar channel of the single-crystal solution Re — 0.4 at.%. of ^{13}C. Some specific features of the γ-quantum yield of the reaction and their dependences on the energy have been established. Electron energy losses of channeling protons have been measured. The γ-quantum yield of the channeling-proton-excited reaction has been demonstrated to depend on the amplitude of thermal vibrations of carbon atoms.

1. Introduction

The main body of data concerning orientation effects at the channeling of positively charged particles with energies of 0.5—10 MeV has been deduced from the analysis of the dependences of the yield of elastically scattered helium ions and protons on their energy, the angle of the particle entering into a channel, the charges of the crystal atoms and the channeled particle, the lattice type, the crystallographic direction, etc. [1]. It has been shown (see the reference list in work [2]) that if particles channel in the near-surface region (1500—2000 Å) of the crystal, a fine structure, whose characteristic features contain a new information concerning the flux distribution of channeling particles and the properties of the crystalline matrix, emerges in their scattering spectra.

The accuracy of the results obtained in the course of studying the indicated spectral structure is determined first of all by the energy resolution ability of the method applied. The energy resolution of the backscattering method depends on the monochromaticity of particles in the beam that falls onto the crystal, the energy straggling as the particles move in the crystal, and the energy resolution ability of a spectrometer. These reasons confine the energy resolution and inevitably result in smoothing the spectra, smearing their structures, and, as a consequence, in difficulties while interpreting the measurement results [3]. If one deals with the near-surface region of the crystal, the greatest error is contributed to the results of measurements carried out within this method by a spectrometer.

In order to study the fine structure of the spectra of channeling ions, we proposed a new approach [4] which takes advantage of the emission yield of "narrow" isolated resonances that are excited by channeling particles at the nuclei of interstitial or substitutional impurity atoms positioned at definite sites in the crystal [5] and/or at the nuclei of crystal lattice atoms. This method avoids the influence of the energy resolution of a spectrometer on the measurement results, which increases the accuracy of the obtained experimental data. As a result, there appear the additional opportunities to study the formation features of the flux of channeling particles. Basing on the approach proposed, new techniques for determining the electron energy losses of channeling particles and the amplitudes of thermal vibrations of impurity atoms in the crystal have been developed.

To analyze the capabilities of the suggested approach in studying the orientation effects numerically and to determine the values of various physical quantities from experimental data, a computer program for simulating the trajectories of channeling particles and calculating the yield of resonance γ-quanta in the nuclear reaction has been developed.

2. Peculiarities of the Yield of Resonance Nuclear Reactions Excited by Channeling Particles

In the method of the isolated resonance, in order to determine the distribution profile of the impurity element, the yield of reactions, e.g., (p,γ) ones, and the intensity of emission are measured simultaneously as the energy of bombarding particles is varied by small increments [6–8]. The depth, at which the resonance occurs in a polycrystalline medium, depends on the initial energy of particles and bremsstrahlung losses. The amplitude of the reaction yield is proportional to the concentration of impurity atoms at the reached distance.

If the resonance is excited by channeling particles (Fig. 1), the situation changes. The emission yield depends not only on the concentration of impurity atoms, as it does in the case of a polycrystalline target, but also on the crystallographic direction, the arrangement of reacting atoms in the crystal, the angle at which particles enter into a channel, the electron density distribution in the channel, and other factors.

In Fig. 1,*a*, we show the trajectories of protons simulated in the case where the particle beam enters into the channel along the atomic planes of the crystal. Subjected to repulsion forces from the atoms located in the planes, the particles oscillate; the flux of protons becomes redistributed; the areas of loosening and tightening of trajectories emerge. Suppose that the impurity atoms, at which the reaction is excited, are located at regular intervals in the middle plane of the channel. Obviously, the probability of the collision of channeling particles with an impurity at the depth x, where the resonance happens, depends on the distribution of the particle flux over the cross-section of the channel. The reaction yield will be maximum if the particles that enter into the channel with the energy $E_p > E_{\rm res}$ become decelerated in such a way that their energy would reach $E_{\rm res}$ at a distance, where the flux density at the channel midst is maximum.

Therefore, provided the atoms, at which the resonance reaction is excited, are regularly distributed and occupy the known positions in the crystal, the measurement of the dependence of the reaction yield on the initial energy (Fig. 1,*b*) allows one to determine the flux distribution of channeling particles and to investigate its dependence on the lattice type, the crystallographic direction, bremsstrahlung losses of energy, the angle, at which particles enter into the channel, and other factors.

In this case, one has to register the number of interactions which stimulated the emission, rather than the energy of reaction products. Therefore, the influence of a spectrometer is excluded. The influence of the straggling at the initial part of a trajectory is also avoided. As a result, the depth resolution of the isolated resonance method is substantially better than that obtained in the scattering method [7, 8].

A substantial enhancement of the resolution ability of the resonance reaction method in comparison with that of the scattering one opens up fresh opportunities for researches. In particular, this allows one to approach the investigation of orientation effects from another side, namely, to reveal a fine structure in the flux of particles that channel near the crystal surface, to estimate the amplitude of thermal vibrations of impurity atoms in the lattice, to determine the electron energy losses of channeling particles, and so on.

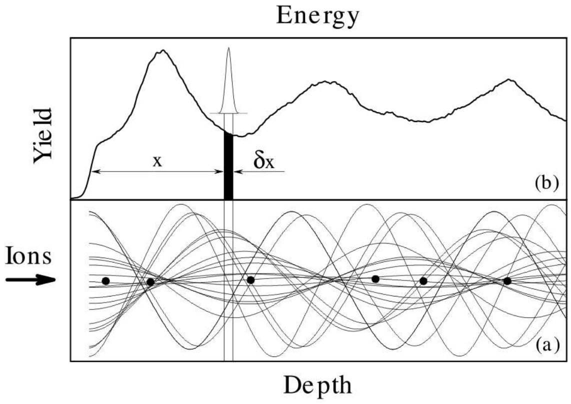

Fig. 1. Concept of measurements of the dependence of the resonant nuclear reaction yield on the energy of ions: (*a*) the distribution of particle trajectories in the planar channel $\varphi_{\rm in} = 0$; (*b*) the yield of γ-quanta of the resonance reaction occurring at the nuclei of impurity atoms located in the middle of the channel (marked by dark circles in panel *a*)

Earlier, narrow isolated resonances have not been used for studying the features of the particle flux redistribution in crystals neither at the axial nor at planar channeling.

3. Dependence of the Yield of the Resonance ^{13}C(p,γ)^{14}N Reaction on the Energy of Channeling Protons

A single-crystal solution Re—0.4 at.%. of ^{13}C was used as the experimental object. As was mentioned above, if the method of resonance under the channeling is used, one has to know the positions of impurity atoms in the crystal lattice.

Interstitial atoms, provided that their concentration does not exceed the solubility threshold, occupy quite definite, energetically beneficial positions in the crystal lattice. In metals with hexagonal close packing (HCP) lattices, the most typical positions, which interstitial atoms can occupy, are octa- and tetrahedral voids. The methods of nuclear physics, together with making use of particle channeling and orientation effects, allow the arrangement of interstitial atoms in the crystal to be

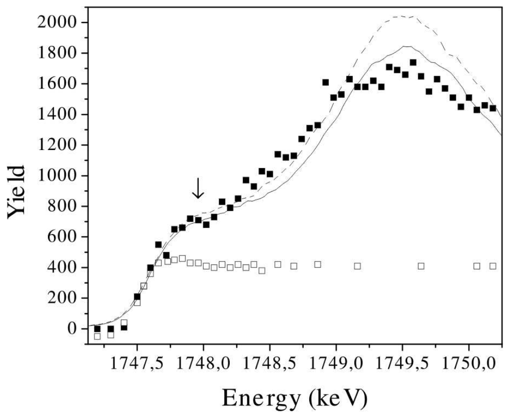

Fig. 2. Excitation functions of the $^{13}C(p,\gamma)^{14}N$ reaction. Experimental results: the yields stimulated by protons channeling along the (0001) plane (solid squares) and by a beam of protons disoriented with respect to the crystal (hollow squares). Theoretical calculations for protons channeling along the (0001) plane and various values of the mean-square amplitudes of thermal vibrations of carbons: 0.102 (solid curve) and 0.09 Å (dashed curve)

measured directly with an accuracy of not worse than 0.1 Å [9].

The fabrication, treatment, and studies of specimens of Re single crystals that contained 0.4 at.% of isotope ^{13}C were described in work [10]. It was also shown there that carbons occupy octahedral voids in rhenium.

Figure 2 exhibits the experimental and theoretical dependences of the γ-quantum yield in the $^{13}C(p,\gamma)^{14}N$ reaction on the initial energy of protons. The strong isolated resonance of this reaction ($E_{\rm res}$ = 1.7476 MeV, $\sigma_{\rm res} \approx 300$ mbarn, $\Gamma_{\rm res} = 135$ eV) was used [11]. At $E = E_{\rm res}$, the drastic increase of the γ-quantum yield was predictably observed, irrespective of crystal orientation. The yield of non-channeled protons (hollow squares) saturates and remains constant irrespective of their energy. It means that only a single resonance and ^{13}C atoms, which are distributed uniformly in the crystal, are excited within the limits of the investigated energy interval. The increase of the yield by more than twice, when particles channel along the (0001) direction (solid squares), testifies to that carbons in rhenium become interstitial impurities.

4. Trajectory Simulation for Protons Channeling in the (0001) Plane of a Single Crystal Re—0.4 at.% of ^{13}C

The computer simulation program that had been developed earlier [12] and the results of the experimental determination of carbon positions in rhenium were used for calculating the evolution of proton trajectories and the yield of γ-quanta in the planar (0001) channel of rhenium. The input parameters of the program were the characteristics of the nuclear resonance of the $^{13}C(p,\gamma)^{14}N$ reaction at an energy of 1.7476 MeV, the characteristics of the planar (0001) channel in the rhenium crystal, and the characteristics of the impurity atoms. The angle between the direction of the beam momentum and the (0001) plane was supposed constant and equal to $\varphi_{\rm in} = 0$. The angular divergence of the beam was taken $\Delta\varphi_{\rm in} \approx 0.03°$. The energy spread of protons in the beam was supposed not to exceed 200 eV.

In order to calculate the force that acts on a proton in the channel, a thermally modified approximation of the averaged potential in the Moliere form was used. The potential created by four planes nearest to a channeling particle was taken into account.

In crystals with a HCP lattice, which rhenium belongs to, there are the same numbers of octainterstitials and the matrix atoms. In the (0001) direction, the planes of rhenium atoms alternate with those of octainterstitials. Moreover, the latter which include carbons are positioned half way between the former.

The trajectories of several tens of protons in the (0001) channel are depicted in Fig. 3. As the amplitude of the trajectory wave grows, its wavelength decreases. The steepness of trajectories depends on the distance between their enter points into the channel and the nearest plane. Nothing confines channeling protons from collisions with ^{13}C nuclei which are located at octainterstitials (dark circles in the middle of the channel). Moreover, the probability for protons to collide with these atoms increases along the motion path due to the redistribution of the proton flux in the channel [9].

Near the middle plane of the channel, where ^{13}C atoms are located, the potential depends weakly on the distances to the crystal planes. Therefore, protons move with small amplitudes of oscillations — practically, in the octainterstitial planes. Their motion in this region is governed by their energy losses at valence electrons. Near the surface, before the first node, the trajectories form a "quasi-cone". Near the cone's axis, the proton flux remains constant on average. Therefore, one may expect for the appearance of a "plateau" in the dependence of the γ-quantum yield on the proton energy.

The proton scattering by thermal oscillations of atoms in the planes and by electrons, as well as the anharmonicity of the potential, results in the entangling of particle trajectories in the channel at large depths.

Figure 2 depicts the experimental and theoretical functions of reaction excitation before the first trajectory node in the (0001) plane. In the case of channeling, the yield of γ-quanta grows with the energy of protons. This excitation function has a 400-eV "plateau" (marked by an arrow in Fig. 2). Here, the yield of γ-quanta in the reaction is close to a constant value, being considerably larger than that for non-channeling protons. The results of simulations showed that the yield of these γ-quanta is caused by protons with low transverse energies which oscillate within the limits of thermal vibrations of ^{13}C atoms. Under planar channeling, we call these protons hyperchanneling.

The excess of the yield of γ-quanta stimulated by hyperchanneling protons over that stimulated by a disoriented proton beam is caused by the reduction of the electronic bremsstrahlung losses of those protons, the trajectories of which transverse the shell of valence electrons. The estimations carried out for this case showed that $(dE/dx)_{\rm cnl}/(dE/dx)_{\rm rnd} \approx 0.64$. Thus, we have a new method for the determination of the electron energy losses of hyperchanneling particles.

The simulation program considers thermal vibrations of impurity atoms in the transverse plane of the channel in the harmonic approximation. The numerical calculations showed (Fig. 2) that the reaction yield at the maximum of the excitation function depends on the amplitude of thermal oscillations of a carbon. This result is explained by the redistribution of the proton flux, which leads to the formation of the first trajectory node (Fig. 3) and to the maximum in the yield of γ-quanta (Fig. 2). Being subjected to forces, protons are focused in a small region of space (about of 0.30 Å) located in the plane of ^{13}C atoms. The probability of the reaction depends in this case on the probability of the ^{13}C atom dwelling in the node vicinity. As the amplitude of vibrations increases, the carbon spends more time beyond the specified region. As a result, the probability of the reaction and, therefore, its yield diminish. For the experimental data presented in Fig. 2, the best agreement is obtained if the value of the mean-square amplitude of thermal vibrations of ^{13}C atoms is equal to 0.102 Å which is several times larger than the mean-square amplitude of thermal oscillations of Re atoms.

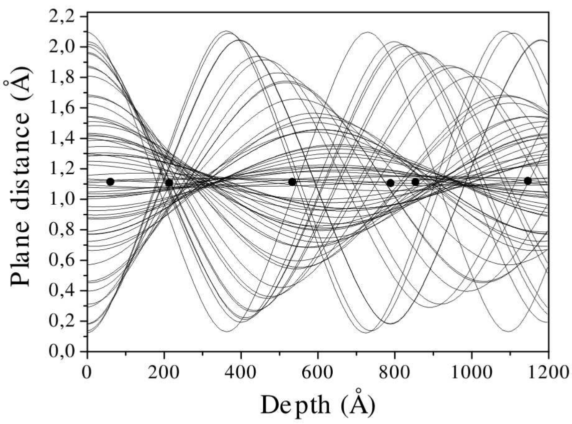

Fig. 3. Oscillations of the trajectories of protons with an initial energy of 1.7476 MeV in the planar (0001) channel of crystals Re—0.4 at.% of ^{13}C. $\varphi_{\rm in} = 0$. Dark circles mark ^{13}C atoms in the interstitial plane in the middle of the channel

5. Conclusions

The isolated resonances of reactions occurring at the nuclei of impurity atoms, which occupy definite positions in the crystal, have been used for the first time to study orientation effects. The fine structure of the reaction excitation function for the proton channeling in the (0001) planar channel of the crystal Re–0.4 at.% of ^{13}C has been studied. The method for determination of electron bremsstrahlung energy losses of channeling protons which move within the limits of thermal vibrations of impurity atoms has been proposed. It has been determined that $(dE/dx)_{\rm cnl}/(dE/dx)_{\rm rnd} \approx 0.64$ in the planar (0001) channel of the crystal Re—0.4 at.% of ^{13}C. The yield of the resonance reaction that is excited by channeling particles has been demonstrated to depend on the amplitude of thermal vibrations of interstitial atoms. The value obtained for the mean-square amplitude of thermal oscillations of carbon atoms is equal to 0.102 Å.

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ДОСЛІДЖЕННЯ ОРІЄНТАЦІЙНИХ ЕФЕКТІВ У КРИСТАЛАХ ЗА ДОПОМОГОЮ ІЗОЛЬОВАНИХ РЕЗОНАНСІВ ЯДЕРНИХ РЕАКЦІЙ

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Р е з ю м е

Ізольований резонанс ядерної реакції на прониклих атомах домішок вперше використано для вивчення орієнтаційних ефектів. Резонанс реакції ^{13}C(p,γ)^{14}N при енергії протонів 1,7476 МеВ використано для дослідження розподілу потоку протонів у площинному каналі (0001) монокристалічного розчину Re–0,4 ат.%^{13}C. Встановлено особливості виходу γ-квантів реакції в залежності від енергії. Виміряно електронні втрати енергії каналованих протонів. Показано, що вихід γ-квантів реакції, яка збуджується каналованими протонами, залежить від амплітуди теплових коливань атомів вуглецю.