# Channeling of helium ions in $PrBa_2Cu_3O_{7-\delta}$ single crystals

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The orientational dependence of the yield of Rutherford backscattering of $He^+$ ions from single crystals of $PrBa_2Cu_3O_{7-\delta}$ in the tetragonal phase has been studied. The half-widths of the angular dependences of the Rutherford backscattering yield and the minimum relative yield of the Pr + Ba and Cu sublattices were found to differ markedly during the channeling.

The Rutherford-backscattering (RB) method has recently been used extensively to study high-$T_c$ superconductors. The Rutherford-backscattering spectrum has characteristic steps, from the position and amplitude of which one can determine the mass number and the concentration of the elements which form the compound under study. The chemical state of the substance to be studied does not affect the Rutherford-backscattering spectrum, in which only the nuclei that scatter the incident ions are taken into account. For this reason the RB method is a perfect method for determining the composition of a compound. This method is frequently used to calibrate standards for microprobe x-ray analysis and for other comparative methods.

If the direction of the incident beam relative to the crystal axes is changed gradually, the Rutherford-backscattering yield will decrease rapidly due to channeling if the direction of the beam is the same as that of the principal crystallographic axis.[1] Analysis of the nature of channeling can yield information on the structural inhomogeneities of the crystal (dislocations, twinning planes, etc.) and on the dynamic properties of the sublattices of various atoms which form the crystal structure.

To avoid complications associated with the formation of twinning planes in the orthorhombic phase of high-$T_c$ superconductors of the 1–2–3 type, we chose a perfect tetragonal crystal of $PrBa_2Cu_3O_{7-\delta}$, consisting of $1.5\times1.5\times0.3$-mm wafers with well-developed, mirror-smooth, natural {001} and {100} faces, in order to study the channeling. The crystals were grown by a method of crystallization from a solution in a melt in the $Pr_2O_3$-BaO-CuO system.[2]

The experimental arrangement is shown in Fig. 1. A 3.0-MeV $He^+$ ion beam from an electrostatic accelerator is produced by a system of diaphragms and aimed at a $PrBa_2Cu_3O_{7-\delta}$ crystal in a triaxial goniometer. The beam diameter is $\sim1$ mm and the angular divergence of the beam is no greater than 0.02°. A collinear laser beam is used to control the beam position at the target. The scattered ions are detected by a semiconductor detector with $\sim13$-keV energy resolution. To aovid a distortion of the Rutherford-backscattering spectra when part of the beam strikes the substrate, we placed the sample on a graphite plate whose RB spectrum lies in the low-energy region and does not overlap the spectrum of the heavy components of the sample.

  

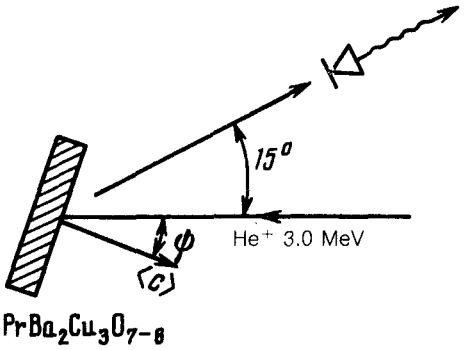


FIG. 1. Experimental arrangement.

The RB spectrum which is measured when the beam strikes the single crystal at a random angle is shown in Fig. 2. The arrows indicate the leading edges of the spectrum which correspond to the scattering by the atoms of the heavy components at the surface. Because the mass of Pr (140.9) is approximately equal to that of Ba (137.3), these elements are hardly discernible in the spectrum, forming a single step. The step due to Cu (63.5) is seen at lower energies. The solid line in Fig. 2 represents a computer-simulated spectrum with the heavy-component ratio Pr:Ba:Cu = 1:2:3. The SANDV program was used in the simulation.[3] This ratio was held for the test crystals

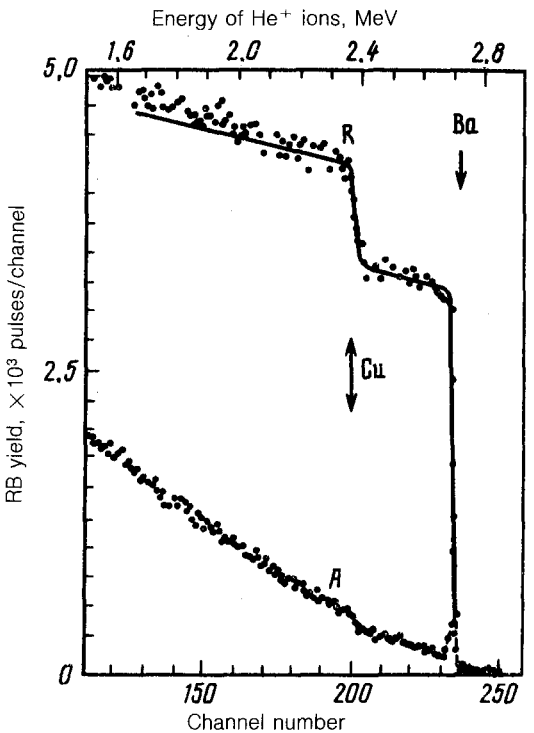


FIG. 2. Rutherford-backscattering spectra for the $PrBa_2Cu_3O_{7-\delta}$ crystal. Spectrum $A$ was measured in the axial (the $\langle c \rangle$ axis) channeling regime and spectrum $R$ was measured in the case of random incidence of the analyzing 3.0-MeV $He^+$ ion beam. (The $\langle a \rangle$ axis runs at an angle of $\sim 15°$ to the plane of the drawing.) The solid line represents the theoretical spectrum calculated under the assumption of random incidence of the beam.

within 10%, as confirmed by the good agreement of the experimental and theoretical spectra.

As we go from a situation in which the beam is incident on the crystal at a random angle (see spectrum *R* in Fig. 2) to a situation in which the beam is incident along the crystallographic ⟨*c*⟩ axis which is perpendicular to the {001} face, the number of backscattered particles decreases sharply because of channeling (see spectrum *A* in Fig. 2).

One of the important characteristics of the crystal which is determined by the channeling method is $\chi_{\min}$, the ratio of the minimum RB yield in spectrum A to the RB yield in the same channel of spectrum *B*. The value of $\chi_{\min}$ measured in this manner is 3.5% that of Ba + Pr sublattice (~230th channel), which is almost 3.2% that of a perfect crystal, calculated on the basis of the model of Ref. 4. This result suggests that the crystal is of a high quality and that its structure is only slightly mosaic. The high quality of the surface layer and the absence of impurities can be deduced from the characteristic of the surface peak (~235th channel) in spectrum *A*, which is caused by the scattering by surface atoms of the crystal. We see from the area under the peak that there are approximately $1.5\times10^{15}$ displaced atoms of Pr + Ba per square centimeter of the crystal surface, which amounts to less than one monolayer.

The results of measurements of the angular dependence of the RB yield at the surface layer (30–50 nm) are shown in Fig. 3. As follows from Fig. 3a, the half-width of the orientational dependence of Rutherford backscattering from a Pr + Ba sublattice is $\psi_{1/2} = 1.0°$.

The spectrum for channeling in the Cu sublattice can be clearly identified by interpolating the RB yield from the Pr + Ba sublattice in the region where the RB spectrum is superimposed on Cu. We thus see that $\chi_{\min}$ (Cu) = 16.0% for the channeling in the Cu sublattice is much larger than that for the channeling in the Pr + Ba

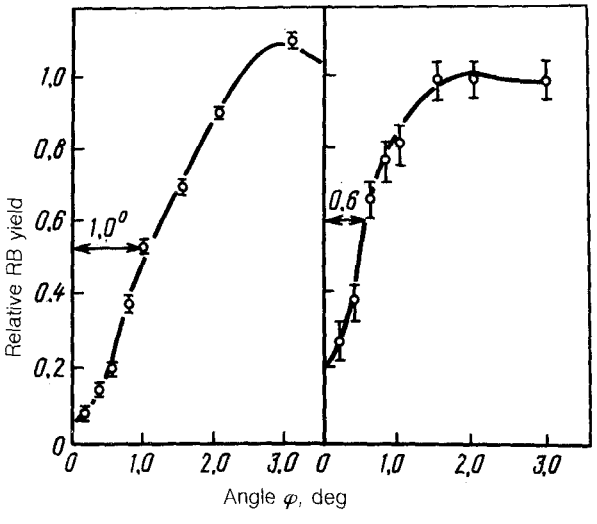


FIG. 3. Orientational dependence of the RB yield in the surface layer at a depth of ~30–50 nm for the Pr + Ba sublattice (a) and Cu sublattice (b).

sublattice. The half-width of the angular dependence of the Rutherford backscattering from the surface Cu atoms, $\psi_{1/2}(\mathrm{Cu}) = 0.6°$, is considerably smaller than that of the Pr + Ba sublattice.

Stoffel *et al.*,[5] found that the width of the orientational dependence for the Cu sublattice also decreases in $YBa_2Cu_3O_x$ crystals which have the same structure as $PrBa_2Cu_3O_x$ (Ref. 6). The half-widths obtained by us, $\psi_{1/2} \approx 1°$ and $\psi_{1/2} \approx 0.6°$, respectively, for the Pr + Ba and Cu sublattices are in good agreement with the critical angles $\psi_1 = 0.96°$ and $\psi_1 = 0.69°$ which were estimated from the Lindhard formula[1]:

$$\psi_1 = (2Z_1Z_2e^2/Ed)^{1/2},$$

where $Z_1$ is the charge of the analyzed ions, $Z_2$ is the average nuclear charge of the atomic chain in the sublattice, $E$ is the particle energy, and $d$ is the atomic spacing in the chain.

The higher value of $\chi_{\min}$ for the Rutherford backscattering from a Cu sublattice than for the Pr + Ba sublattice correlates with the strong anisotropy of the thermal vibrations of the Cu atoms in the $PrBa_2Cu_3O_x$ crystal. In the Cu1 position their vibration amplitudes in the plane perpendicular to the $\langle c \rangle$ axis are much higher than those along this axis.[6] This particular feature is less clearly defined in the case of copper atoms in the $YBa_2Cu_3O_x$ crystal.[6]

In summary, we have studied for the first time the channeling in single crystals of $PrBa_2Cu_3O_{7-\delta}$ and we determined separately for the Pr + Ba and Cu sublattices the angular dependence of the Rutherford-backscattering yield. The half-widths $\psi_{1/2}$ and the minimum relative yield $\chi_{\min}$ of these sublattices were found to be different. This difference can be attributed to the considerably higher amplitude of the thermal vibrations of Cu atoms in the plane perpendicular to the $\langle c \rangle$ axis in the $PrBa_2Cu_3O_{7-\delta}$ lattice.


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