controlled by the O atom modulation in the CuO_2. We have further investigated the temperature dependence of the atomic modulations in $Sr_{14}Cu_{24}O_{41}$, particularly in the CuO_2 chain in which the spin-gap behavior accompanied by the formation of the spin-dimerized state is realized at low temperature. By single-crystal x-ray-diffraction method, we have confirmed that superspace group of the modulated structure remains unchanged from room temperature to 150K. The hole distribution has been considered on the basis of the changes of lattice constants, the atomic modulation and the interatomic distances between Cu in the Cu_2O_3 and O atom in the CuO_2. It is indicated that the small amount of holes doped in the Cu_2O_3 have been back-transferred to the CuO_2 and that almost all of the holes are localized in the CuO_2 at low temperature. Moreover, the possible hole-ordered structure with the Zhang-Rice singlet in the CuO_2 are mainly due to the O atom modulation in the CuO_2 and the ZR-singlet site with rectangular CuO_4 unit is possible in the CuO_2, which is analogous to the local CuO_4 coordination in the CuO_2 plane of high-T_c cuprates.

Keywords: superconductor oxides, composite crystals, incommensurate modulated structures

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Structural study on the rattling phenomena in the β -pyrochlore oxides and filled skutterudites

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β-pyrochlore oxides and filled skutterudites exhibit a wide variety of physical properties; superconductivity, heavy fermion, valence fluctuation, non-Fermi liquid behavior. The alkali ions in the β -pyrochlore oxides and the rare earth ions in filled skutterudites are located inside the oversized cages, and these ions are rattling heavily with large thermal displacements. In order to elucidate the relation between the rattling and the physical properties, we carried out X-ray diffraction measurements on single crystals of β-KOs_2O_6 and $NdOs_4Sb_{12}$ using a CCD area detector and a curved imaging plate. It is known that the two compounds exhibit the largest rattling among each series. The values of the atomic displacement parameter U_{eq} are estimated at U_{eq}=0.0735(8) for K in β-KOs_2O_6 (Fd-3m) and U_{eq}=0.0558(1) for Nd in $NdOs_4Sb_{12}$ (Im-3) at 300 K, which are significantly large in comparison with the other atoms. It is found that the electron density of the K atom in β-KOs_2O_6 is not spherical but extended considerably along the <111> direction in spite of the high point symmetry of the site (-43m), giving evidence for a large anharmonic vibration of the K atom. In contrast, the Nd atom in $NdOs_4Sb_{12}$ shows isotropic electron density, consistent with the m-3 site symmetry. Thus, it is concluded that the anharmonicity, which is the key issue for the rattling, is more pronounced in β-KOs_2O_6. In addition, on the first-order transition for β-KOs_2O_6 at T_p = 7.5 K below the superconducting transition at T_c = 9.6 K, we found a clear stepwise change in the X-ray intensity of some selected reflections, which must be relevant to some sort of changes in the rattling of the K atom.

Keywords: structural studies, superconducting materials, heavy fermions

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Microstructure and superconductivity in polycrystalline boron-doped diamonds

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The discovery of superconductivity in polycrystalline boron-doped diamond (BDD) synthesized under high pressure and high temperatures (Ekimov et al. (2004) Superconductivity in diamond. Nature 428: 542) has raised a number of questions on the origin of the superconducting state. It was suggested that the heavy boron doping of diamond eventually leads to superconductivity. To justify such statements a more detailed information on the microstructure of the composite materials and on the exact boron content in the diamond grains is needed. For that we utilized high-resolution transmission electron microscopy as well as electron energy loss spectroscopy. For the studied superconducting BDD samples synthesized at high pressures and high temperatures the diamond grain sizes are about 1-2 microns with a boron content between 0.2(2) and 0.5(1) at.%. The grains are separated by 10-20 nm thick layers and triangular-shaped pockets of predominantly (at least 95 at.%) amorphous boron. Our results render superconductivity caused by the heavy boron doping in diamond highly unlikely.

Keywords: superconducting materials, microstructure, TEM characterization

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Superconductivity and charge-density wave in ring- or Moebius-shaped $NbSe_3$ and TaS_3 single crystals

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$NbSe_3$ and TaS_3 single crystals of ring- or Moebius-shape have been fabricated by Tanda et al. and an intriguing possibility to investigate superconductivity or charge-density wave (CDW) in these topological spaces has been opened. In this paper, we predict several new phenomena in these systems based on both phenomenological Ginzburg-Landau theory and microscopic Bardeen-Cooper-Shrieffer theory. First we study the physical properties of superconductivity in a Moebius ring, which is obtained by applying pressure or doping atoms to $NbSe_3$. Most interesting phenomenon appears when a magnetic field is applied to this system: an ordinary Little-Parks oscillation, which is an oscillation of transition temperature as a function of magnetic flux (F) threading the ring, is modified especially when F is close to a half-odd-integer times a superconducting magnetic flux quantum, and novel superconducting states appear which have a gap node along the center line of the Moebius ring. This kind of state has never been achieved in other