controlled by the O atom modulation in the CuO$_2$. We have further investigated the temperature dependence of the atomic modulations in Sr$_2$Cu$_2$O$_6$, 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 CuO$_2$ and O atom in the CuO$_2$. It is indicated that the small amount of holes doped in the CuO$_2$ 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

P11.01.04

Structural study on the rattling phenomena in the $\beta$-pyrochlore oxides and filled skutterudites

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$\beta$-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 $\beta$-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 $\beta$-K$_2$O$_6$: Sb$_2$O$_6$ and Nd$_2$O$_3$:Sb$_2$ 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 $U_{\parallel}$ are estimated at $U_{\parallel}=0.0735(8)$ for K in $\beta$-K$_2$O$_6$:Sb$_2$O$_6$ (Fd-3m) and $U_{\parallel}=0.0558(1)$ for Nd in Nd$_2$O$_3$:Sb$_2$:O$_6$ (Im-3) at 300 K, which are significantly large compared with the other atoms. It is found that the electron density of the K atom in $\beta$-K$_2$O$_6$:Sb$_2$O$_6$ 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 Nd$_2$O$_3$:Sb$_2$:O$_6$ 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 $\beta$-K$_2$O$_6$:Sb$_2$O$_6$. In addition, on the first-order transition for $\beta$-K$_2$O$_6$:Sb$_2$O$_6$ at $T_s = 7.5$ K below the superconducting transition at $T_s = 9.6$ 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

P11.01.05

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 (Ekmov 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 claims, 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$_2$. Next, we study the physical properties of superconductivity in a Moebius ring, which is obtained by applying pressure or doping atoms to NbSe$_2$. 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
geometries. We also studied the CDW properties in ring-shaped crystals. In this case, the “mixed state” of CDW analogous to that in type-II superconductors is expected which may show quite different electric response from ordinary CDW state. We also comment on some crystal properties of these “topological crystals”.

Keywords: superconductivity, charge density waves, topology

Relaxation of geometrical frustration in NbSe₃

topological crystals

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Geometrical frustration in a curved crystal is examined through synchrotron X-ray diffraction experiments. Also its effects on the material’s charge-density (CDW) ordering are discussed. We performed diffraction measurements on individual NbSe₃ topological crystals, which are µm-scale crystals characterized by their multiconnected topologies. Our samples include rings, a Möbius strip and 2π-twisted strips. Their volume-averaged strain turned out unexpectedly low for such highly deformed crystals, while strain distribution is as broad as >0.01. These features are common to all samples, regardless of their apparent size nor deformation. On the contrary, CDW transition temperatures in crystals with a twist exhibit substantial reduction of a few K, while those without twists showed much less reduction. Also, we have an indication of dimensional crossover in the behavior of pre transition fluctuations between twisted and untwisted samples. We analyzed elastic free energy of topological crystals. A structural model, in which the crystal lattice forms a spiral, best accounts for the measured distribution of lattice strain. According to our model, geometrical frustration due to curvature brings fragmentation of coherent region of atomic arrangements. As a result, enhanced low-dimensionality modifies transition temperatures and pre-transition fluctuations of CDW, in accordance with the transport study.

Keywords: charge density waves, diffraction synchrotron radiation microcrystals, crystal morphology

New class of topological crystals: Hopf link of crystals

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Exotic topological crystals, such as ring-shaped crystals, Möbius strips of crystals, and figure-8 (2π-twisted strip) crystals, have been successfully created in NbSe₃ despite their inherent crystal rigidity by Hokkaido University group [1]. Recently, we discovered new topological crystals of TaSe₃, which are two ring-shaped crystals linked to each other exactly at once [2]. Since the rings are topologically linked, they cannot be removed without cutting of chemical bonding. The topology of the crystal form is called a “Hopf link”, which is the simplest link involving just two component unknots linked together exactly once. Crystallography including the topological crystals has provided rich interesting problems involving their growth mechanism, frustration of defect creations and bending and twisting, topological classification of crystals using concept of manifold embedding and analogous between crystals and general theory of relativity. [1] S. Tanda, T. Tsuneta, Y. Okajima, K. Inagaki, K. Yamaya, and N. Hatakenaka, Nature 417, 397 (2002). [2] T. Matsuura, M. Yanamaka, N. Hatakenaka, T. Matsuayama, and S. Tanda, Journal of Crystal Growth 297, 157-160 (2006).

Keywords: topological crystals, Hopf link, catenane

Polyhedral topological-crystals in TaS₃

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We produced micrometer-scale polyhedral ring-crystals of TaS₃, which are synthesized by chemical vapor transportation method. Topological crystals of MX₂ (NbSe₃, TaSe₃ et al), known as ring and Möbius shaped, is already known since 2000 but angularity of ring-crystal is freshly discovered in TaS₃. The crystals are investigated by electron backscatter diffraction pattern technique and it is revealed that the orientation change abruptly along the circumference. The difference between usual and polyhedral ring-crystals is the arrangement of edge dislocations. Dislocations cause attraction and repulsion by the distance between them. The corner of polyhedral crystal is made by the concentrated dislocations because of attractive interaction between dislocations. Figure (a) shows polyhedral ring-crystals as a result of attractive interaction and (b) shows ring crystals as a result of repulsive interaction. In fabricated various crystals, we insist that these structures are classified by the radius and the thickness.

Keywords: topology, polyhedra, incommensurate structures