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

P11.01.06

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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

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

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Relaxation of geometrical frustration in $NbSe_3$ topological crystals

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Geometrical frustration in a curved crystal is examined through syncrotron X-ray diffraction experiments. Also its effects on the material's charge-density-wave (CDW) ordering are discussed. We performed diffraction measurements on individual $NbSe_3$ topological crystals, which are μm-scale crystals characterized by their multiconnected topologies. Our samples inclede rings, a Mobius strip and 2π-twisted strips. Their volume-avaraged 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 fructuations between twisted and untwisted samples. We analyzed elastic free energy of topological crystals. A structural model, in whichthe 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

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Polyhedral topological-crystals in TaS_3

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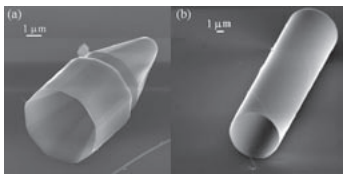
We produced micrometer-scale polyhedral ring-crystals of TaS_3, which are synthesized by chemical vapor transportation method. Topological crystals of MX_3 ($NbSe_3$, TaS_3 et al), known as ring and Moebius shaped, is already known since 2000 but angularity of ring-crystal is freshly discovered in TaS_3. 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

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New class of topological crystals: Hopf link of crystals

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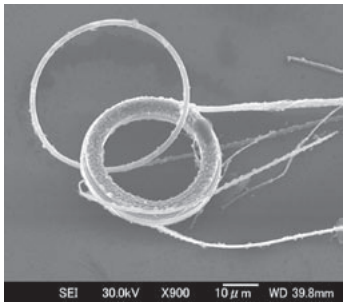
Exotic topological crystals, such as ring-shaped crystals, Mobius strips of crystals, and figure-8 (2π-twisted strip) crystals, have been successfully created in $NbSe_3$ despite their inherent crystal rigidity by Hokkaido University group [1]. Recently, we discovered new topological crystals of $TaSe_3$, 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.



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Keywords: topological crystals, Hopf link, catenane