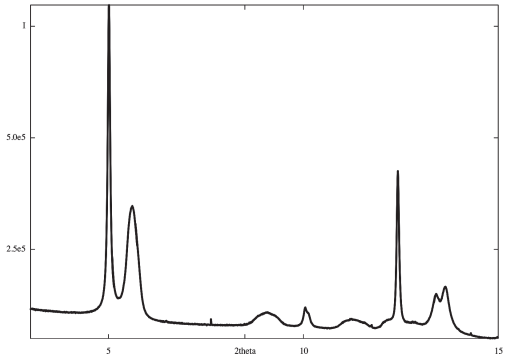
A phenomenological model, based on strongly anisotropic strain, fits well the pattern but provides no structural insight. In fact, the resulting nonconvex strain isosurfaces are unphysical and must be attributed to some other displacive disorder phenomenon. Turning the tables, we chose the Debye Function Analysis (DFA) method [3] – a bottom-up method for modeling powder diffraction patterns based on the set of interatomic distances – to study different disorder phenomena as possible causes. Within DFA the interatomic distances distribution can be modified so as to include *whole canonical ensembles* of atomic configurations, that is a great advantage when considering stochastic models of disorder. Moreover, the interplay of displacive disorder with size/shape and chemical disorder is intrinsically considered. Reverse Monte Carlo methods can also be combined effectively within this method.

We have considered different phenomena to arrive to a comprehensive understanding of this peculiar disorder model in detail, including size/shape, coherent twinning, antiphase domains and Markov-chain anisotropic paracrystallinity based on nearest-neighbor displacement correlations [4]. A detailed analysis of the structural ordering phenomena in $[Ru(CO)_4]_n$ is presented. This work was supported by Fondazione CARIPLO (2009-2446).



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Keywords: total scattering, paracrystal, metal-organic framework

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High-pressure synthesis, structure and properties of novel superhard phases

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The growing demand for advanced superhard materials simulated the search for novel high-pressure phases that are more thermally and chemically stable than diamond and harder than cubic boron nitride (cBN). Following the discovery of diamond-like BC_2N [1] and BCN [2], very recently a number of new superhard phases has been synthesized.

New high-pressure form of elemental boron, orthorhombic γ-B_{28} theoretically predicted by Oganov [3] has been synthesized from high-purity β-B_{106} in the 12-20 GPa range at temperatures above 1800 K. The cell parameters resulting from the Le Bail refinement are a = 5.056(1) Å, b = 5.641(1) Å, c = 6.995(1) Å and R_{wp} = 2.46 %. γ-B_{28} is the least compressible form of elemental boron (B_0 = 237 GPa [4]) and has Vickers hardness of 50 GPa [5], which is higher than the hardness of other boron polymorphs.

A new metastable high-pressure phase, diamond-like BC_5 (d-BC_5), has been synthesized by phase transformation of graphite-like B–C solid solutions at pressures above 20 GPa and temperatures of about 2200 K [6]. Lattice parameter of d-BC_5 at ambient conditions is a = 3.635(8) Å which is slightly larger than that diamond. According to TEM-SAED data, boron and carbon atoms are homogeneously distributed over the diamond-like crystal lattice not forming superstructures. At high temperatures d-BC_5 demonstrates a clear tendency to segregate into carbon and boron carbide, however, at ambient pressure it has been found to be much more thermally stable (to 1900 K) than nanocrystalline diamond of the same grain size. Among superhard phases, the bulk modulus of d-BC_5 (B_0 = 335 GPa) is exceeded only by the bulk moduli of diamond and cBN. Well-sintered millimeter-sized bulks synthesized in a multianvil press are semi-conductive and exhibit extreme hardness (H_V = 71 GPa) comparable with that of single-crystal diamond and very high fracture toughness (K_{1C} = 9.5 MPa $m^{0.5}$).

New boron subnitride, rhombohedral $B_{13}N_2$ has been synthesized by crystallization from the B–BN melt at 5 GPa [7,8]. The structure of $B_{13}N_2$ belongs to the R-3m space group (a = 5.4585(8) Å, c = 12.253(2) Å) and represents a new structural type produced by the distorted B_{12} icosahedra linked together by N–B–N chains and inter-icosahedral B–B bonds [9]. $B_{13}N_2$ has bulk modulus of 200 GPa [10] and is expected to be superhard with Vickers hardness of 40 GPa [11].

Ultrahard nanocrystalline cubic boron nitride with hardness of H_V = 85 GPa (enhancement up to 100% in comparison with polycrystalline cBN) has been synthesized from graphite-like BN with "ideal random layer" structure at pressures above 20 GPa and moderate (~1770 K) temperatures [12]. The material has extremely high fracture toughness (K_{1c} = 10.5 MPa $m^{0.5}$), wear resistance ($W_H \sim 5.9$) and thermal oxidation stability (to 1450 K).

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Keywords: pressure, temperature, material

MS.19.2

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Amorphization, insertion and reactions in microporous materials at high pressure

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Microporous materials, such as zeolites and aluminum phosphates, exhibit low-density structures built up of corner-sharing tetrahedra (SiO_4, AlO_4, PO_4) and are used extensively as molecular sieves