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The electronic structure and properties of crystals can be calculated *ab initio* with CRYSTAL at different levels of approximation ranging from Hartree-Fock (HF) to Kohn-Sham (KS) Density Functional Theory and including use of hybrid functionals. Expressing the crystalline wavefunction in terms of linear combinations of atomic orbitals (LCAO) allows easy interpretation of the electronic structure and direct comparison with molecular fragments. The release of the code presently distributed, CRYSTAL06 (http://www.crystal.unito.it), enables fully automated and efficient search for minimum energy structures and the computation of a variety of properties including structural, elastic, piezoelectric, dielectric, magnetic and electronic properties, and the simulation of vibrational spectra. Extensive use of symmetry, in both the real and reciprocal space, and low computational requirements make the program efficient and suitable for the study of complex structures with ordinary computer facilities. Recent achievements in the parallelization of the code and use of parallel linear algebra libraries now permit large-scale calculations for systems containing thousands of atoms in the unit cell with good scalability over thousands of processors on High Performance Computers. New developments also involve an efficient implementation of the Coupled-Pertubed (CP) HF/KS equations for the calculation of linear and nonlinear optical properties of insulators and semiconductors (electron polarization, dielectric and hyperpolarizability tensors). Application of the CPHF/CPKS method to the analytical calculation of various properties such as the piezoelectric tensor, infrared and Raman intensities is under development. The new features will be illustrated through examples of application.

Keywords: *ab-initio* periodical and cluster calculations, crystal structure and properties, DFT

MS.38.1

Acta Cryst. (2008). A**64**, C71

Phase field modeling of self-organized polycrystalline structures: Denrites, spherulites, eutectics

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Recent advances we made recently in phase field modeling of polycrystalline self-organized structures will be reviewed. Self-organized crystalline patterns are present in a variety of systems including metals, polymers, minerals, and biological systems. The fact that similar polycrystalline patterns are seen in systems of very different molecular structure suggests that a minimal model based on coarse-grained fields, which neglects details of the molecular interactions, might be feasible. Along these lines, we have developed a phase field models of polycrystalline solidification that rely one or more orientation fields in representing crystallographic orientation. Our models have been applied for describing various self-organized structures including dendritic morphologies, disordered dendrites, spherulites, and eutectic structures in 2D and 3D. Our models consist of several mechanisms for nucleating new grains at the perimeter of the crystallites, including homogeneous and heterogeneous processes. It will be shown that a wide range of observed polycrystalline morphologies can be reproduced by varying only a few model parameters. Preliminary results for modeling dendritic and eutectic self-organization in an atomistic phase field theory (the phase field crystal model) will also be presented.

Keywords: self-organization, phase field theory, polycrystals

MS.38.2

Acta Cryst. (2008). A**64**, C71

High temperature characteristics of unidiectionally solidified ceramic eutectics

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We have recently developed ceramic eutectics, which are named Melt Growth Composites (MGCs). The binary MGCs (Al_2O_3/YAG and Al_2O_3/GAP binary systems) have a novel microstructure, in which continuous networks of single-crystal Al_2O_3 phases and single-crystal oxide compounds (YAG or GAP) interpenetrate without grain boundaries. To characterize the entangled structure of the typical MGCs, the X-ray computerized tomography (micro X-ray CT) was performed at a synchrotron radiation facility Spring8. The micro X-ray CT showed that the Al_2O_3 and the YAG are entangled with each other. Therefore, the MGCs have excellent high-temperature strength characteristics, creep resistance, superior oxidation resistance and thermal stability in the air atmosphere at very high temperatures. In the paper, high temperature characteristics of MGCs such as high temperature strength (Fig. 1), creep resistance, oxidation resistance and thermal stability of microstructure, and structural characteristics of the typical MGCs will be briefly introduced.

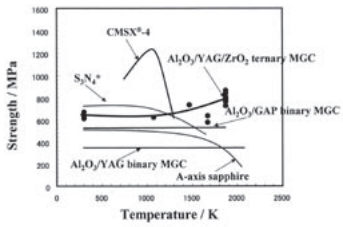

Fig. 1 Temperature dependence of strength of Al_2O_3/YAG, Al_2O_3/GAP binary and Al_2O_3/YAG/ZrO_2 ternary MGCs.

Keywords: high-temperature ceramics, single crystal, mechanical properties

MS.38.3

Acta Cryst. (2008). A**64**, C71−72

Nanoparticle halo formation around colloids in binary solutions

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Colloidal suspensions are widely used in applications such as photonic crystals and coatings, where nanoparticle engineering is a new model whereby interactions may be regulated to provide control over suspension stability. One such stabilizing mechanisms is nanoparticle “haloing.” This colloidal stabilization mechanism has been predicted theoretically and inferred experimentally in microsphere-nanoparticle mixtures that possess high charge and size asymmetry. The term “halo” implies the existence of a non-zero separation between the highly charged nanoparticles and the negligibly charged microspheres that they surround. For the first time, we were able to quantify this nanoparticle-microsphere particle

distance, to determine the average number of nanoparticles associated with each microsphere, and to define the correlations among the nanoparticles in the halos. Our observations, based on ultra-small-angle X-ray scattering, reveal the fundamental nature and structure of the haloing effect, and demonstrate that the nanoparticles are separated from the microsphere by a distance close to the Debye screening length of the solution.

Keywords: colloidal suspensions, photonic crystals, small-angle x-ray scattering

MS.38.5

Acta Cryst. (2008). A**64**, C72

Self-assembled magnetite particles formed 4.6 billion years ago

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We report magnetite colloidal crystals formed in the space 4.6 billion years ago. In the meteorite parent body there were abundant waters, and some minerals were generated as a result of the aqueous alteration. Magnetite (Fe_3O_4) is one of typical minerals formed by the aqueous alteration. We found the colloidal crystals composed of magnetite with various morphologies, e.g. octahedral and rhombic dodecahedral. These morphologies determine the structure of the colloidal crystals: in the case of octahedral morphology, the lattice structure is body centered cubic (BCC), while the lattice structure is face centered cubic (FCC) in the case of rhombic dodecahedral morphology. This relationship was not observed for spherical constituent particles. It is known that a repulsive force between particles is necessary for the formation of colloidal crystals. Magnetite has a magnetic force that results in strong attraction between the particles. It suggests that other particles that have no or weak magnetic force must be the precursor for magnetite colloidal crystal formation. These precursor particles could disperse in solution and subsequently form of the colloidal crystals, finally transformed into magnetite. A possible candidate is greigite, which was observed at the surface of the magnetite particles.

Keywords: colloids, magnetic particles, meteorite

MS.39.1

Acta Cryst. (2008). A**64**, C72

Total scattering: The key to the local and medium range structure of complex materials

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Structural characterization is mainly based on the measurement of Bragg intensities and yields the average structure of the crystalline material. However, this approach ignores any defects or local structural deviations that manifest themselves as diffuse scattering. It also fails in case of disordered materials, badly crystalline such as many nano-materials, or not crystalline at all, such as glasses. In some cases crystalline and amorphous phases coexist making the traditional crystallographic structure refinement difficult or incomplete. The total scattering pattern, however, contains structural information over all length scales and can be used to obtain a complete structural picture of complex materials. Suddenly one has access to a new parameter, the real-space range of the refinement and structures can be analyzed as function of length scale straight forwardly. Here we present different applications of this technique including data taken on the high resolution neutron powder diffractometer NPDF located at the Lujan Neutron Scattering Center at Los Alamos National Laboratory. This instrument is design for total scattering studies using the Pair Distribution Function (PDF) approach and length scales in excess of 200A can be accessed.

Keywords: total scattering, disordered materials, neutron powder diffraction

MS.39.2

Acta Cryst. (2008). A**64**, C72−73

New opportunity to explore noncrystalline materials by neutron total diffractometer (NOVA) at J-PARC

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A neutron total diffractometer, named “NOVA”, is constructing now at Japan Proton Accelerator Research Complex (J-PARC). NOVA will be used as very intense powder diffractometer since