# MM 20: Poster Session I

Time: Tuesday 14:45–16:30 Location: P4

MM 20.1 Tue 14:45 P4

**Radiotracer Diffusion of Iron and Phosphorus in Sintered Iron Powders** — •Deniz Yüksel, Sergiy Divinski, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Germany

Many technological applications require materials with both, good magnetic properties, e.g. fast change of polarisation and high magnetic saturation, and excellent mechanic properties, i.e. large Vickers hardness and high tensile yield stress, at the same time. A strategy for obtaining such beneficial property combination at reasonable materials costs is based on alloying of iron with phosphorus and silicon. We applied a powder metallurgical route for initial materials synthesis. The metal powders were then compacted and sintered. In order to optimize the sintering process, the diffusion kinetics of iron and particularly of the alloying elements has to be known. We investigated the diffusion of $^{59}$Fe and $^{32}$P in sintered Fe-P materials as a function of the sintering parameters. The results are discussed with respect to the applicability of the alloys for magnetic applications.

MM 20.2 Tue 14:45 P4

**Schadensvorhersage an vordeformiertem und wechselbelastetem Karbonstahl** — •Patrick Eich, Matz Haaks und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Die Vorhersage der Lebensdauer von Bauteilen unter zyklischer Belastung basiert bis heute auf der 150 Jahre alten Wöhlermethode. Ein aussagefähiges Wöhlerdiagramm erfordert Lastzahlen von $10^8$ bis $10^9$ und eine große Anzahl äquivalenter Proben. Damit ist sie sehr zeit- und kostenintensiv. Die Positronen- Annihilations- Spektroskopie (PAS) bietet eine neue Methode der Schadensvorhersage. Die mikroskopische Ursache der Ermüdung ist die Akkumulation von Gitterfehlern, die selbst bei geringer zyklischer Belastung zum Materialversagen führen kann. Die Defektdichte des Materials kann mithilfe der PAS gemessen werden. Selbst geringe Änderungen der Defektdichte, wie sie zu Beginn der Ermüdung auftreten, lassen sich über die Zerstrahlungsparameter bestimmen und als Vorbote der Ermüdung des Materials heranziehen. Die Zuverlässigkeit dieser Methode konnte für Karbonstahl- und Aluminiumproben mit defektarmem Ausgangszustand bereits gezeigt werden. Da der industrielle Auslieferungszustand eine bestimmte Vorschädigung aufweißt, werden aktuelle Ergebnisse von vordeformierten und anschließend wechselbelasteten Zugproben des Karbonstahls C45E vorgestellt. Die Defektdichte wurde mit der Bonner Positronen Mikrosonde untersucht und als Maß für die Schädigung herangezogen. Die Lebensdauer der Proben konnte dabei bereits aus dem Frühstadium der Ermüdung abgeschätzt werden.

MM 20.3 Tue 14:45 P4

**Diffusion of Gold in Lead Investigated by Neutron Activation Analysis** — •Dirk Böckmann and Nicolaas Stolwijk — Universität Münster, Institut für Materialphysik, 48149 Münster

Fast impurity diffusion in lead has been extensively studied in the 1960s and 1970s. In this context, Pb:Au served as a prototype system. In particular, it was concluded from measurements of Pb self-diffusion enhancement factors in Pb(Au) alloys that the high Au diffusivity cannot be reconciled with the vacancy mechanism. Alternative models interpreted Au transport in terms of fast moving interstitial-type defects including conventional interstitials $Au_i$, $Au_i$-vacancy pairs, or Au-Au diplons (dumbbells), however, without providing convincing evidence. Specifically, the role of substitutional $Au_s$ was not sufficiently clarified. Our experiments aim at identifying the mechanism of Au diffusion in Pb by looking closely at the concentration dependence and time evolution of the Au penetration profiles. To this aim, we utilise the suitability of the Pb:Au system for neutron activation analysis (NAA), which allows for the detection of diffusion profiles on an absolute concentration scale. First results are discussed within the framework of interstitial-substitutional diffusion involving $Au_i$-$Au_s$ exchange with the aid of vacancies.

MM 20.4 Tue 14:45 P4

**Investigation of point defects in the cathode material $LiCoO_2$: first-principles calculations** — •Melanie Gröting[1], Peter C. Schmidt[2], and Karsten Albe[1] — [1]Materialwissenschaft, TU Darmstadt, Germany — [2]Physikalische Chemie, TU Darmstadt, Germany

$Li_xCoO_2$ has been widely used in rechargeable lithium ion batteries for decades. Still, there exists no comprehensive understanding of the mechanisms that contribute to degradation in these batteries. However, in the commercially applied concentration range 1.0>x>0.5 microstructural changes, redox and intercalation reactions with the electrolyte, and particularly point defects in the active material are believed to play an important role in the degradation process. Knowledge of the energetics of different point defects are therefore mandatory in order to understand this material more properly.

In this study we use density-functional theory calculations (DFT) to investigate the thermodynamic stability of $Li_xCoO_2$ with lithium contents x=1.0, 0.5 and 0.0 with respect to the competing metal oxides. Moreover, the formation energies of several charged point defects in these compounds using the supercell approach are calculated. We take lithium and cobalt vacancies into account, as well as oxygen vacancies and interstitials. Especially the oxygen related defects play an important role, which is also evidenced experimentally by performance improvement on coating of the active material e.g. with alumina. Besides the thermodynamic behavior of the defects also the electronic structures and density of states are examined in order to compare them with XPS data.

MM 20.5 Tue 14:45 P4

**Spin-phonon scattering and heat transport in spin ladders** — •Christina Seidler and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

We study the spin-phonon dynamics and the heat transport of two-leg spin-1/2 ladders in the presence of a magnetoelastic deformation-potential coupling. In the limit of weak inter-rung exchange we employ a mapping of the spin degrees of freedom to a gas of non-interacting bond-bosons to describe the magnetic excitations. The coupled spin-phonon excitations are derived perturbatively and their spectra will be discussed as a function of momentum, frequency, temperature, system parameters and external magnetic fields. Both optical and acoustical phonons will be considered.

The heat transport will be investigated in the linear-response regime by evaluating the corresponding Kubo integrals. Results for the temperature and the magnetic field dependence of both, the magnetic and phononic heat conductance, will be presented. In particular the effect of the field-induced triplet softening will be regarded.

Our results will be put into the context of the anomalous magnetic heat transport of the spin-ladder compound $Sr_{14}Cu_{24}O_{41}$.

MM 20.6 Tue 14:45 P4

**Characterization of the Brittle-to-Ductile Transition in NiAl Single Crystals** — •Michael Scharnweber, Carl-Georg Oertel, and Werner Skrotzki — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden

Hard oriented NiAl single crystals (<100> deformation axis) have been deformed in compression above and below the Brittle-to-Ductile Transition Temperature (BDTT). The investigation of slip lines suggests a smooth transition from {112}<111> slip at 550 K to {110}<110> slip at 620 K. However, the results of the compression experiments reveal a rather sharp transition in the temperature range 645 K - 655 K. Below the BDTT an anomalous temperature dependence of the yield stress was observed. The activation enthalpy measured supports the deformation model given by Mills et al. [1] suggested for {110}<110> slip. For comparison, soft oriented single crystals (<110> deformation axis) have been deformed in the same temperature range. The active slip system found was {100}<100> with the faint slip line pattern indicating cross slip. For <110> orientation in the whole temperature range investigated the yield stress decreases with increasing temperature.

[1] M.J. Mills, R. Srinivasan, M.S. Daw, Phil. Mag. A, 77, 801 (1998)

MM 20.7 Tue 14:45 P4

**How to apply a simulation of field evaporation of intermetallic phases to extract material parameters** — •Torben Boll and Talaat Al-Kassab — Institut für Materialphysik, Georg-August Universität Göttingen, 37077 Göttingen, Friedrich-Hund-Platz 1

In this contribution the authors will present a model of the field evap-

oration process, which is used to reconstruct 3D AtomProbe Tomography (APT) data. The model is based on the commonly used Müller-Schottky-Method to calculate field evaporation field strengths. The simulations are valid for universal formulation and will be focused towards intermetallic phases, such as $L1_0$-TiAl and $L1_2$-$Cu_3Au$ in this presentation. By comparing the results of the simulations with experimental data with the AtomVicinity algorithm material parameters such as the Cu-Au binding energy, the ionization energy or field evaporation field strengths of the respective species can be estimated. Artifacts that are visible in the experimental APT-data can be explained as well. The AtomVicinity algorithm explores the local environment of the atoms and delivers the site occupation of the different species at the respective sublattice positions.

MM 20.8 Tue 14:45 P4

**Analysis of GPB zones of AlMgCu alloys** — •Iris Kohlbach[1], Björn Korff[1], Benedikt Klobes[1], Torsten Staab[2], Matz Haaks[1], and Karl Maier[1] — [1]Universität Bonn, HISKP, Nussallee 14-16, 53115 Bonn — [2]Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg

In contrast to the textbook example AlCu, early precipitation stages of AlMgCu alloys are not well understood. The first structures for early precipitates were proposed by Bagaryatsky in 1952 [1]. He suggested a local atomic order similar to the S-phase. However, this has not been confirmed until today. We studied Guinier-Preston-Bagaryatsky (GPB) zones by a comparison of several experimental und numerical methods. According to Bagaryatsky's original suggestion we calculated total and binding energies of several MgCu structures in the Al-matrix using the ab-initio code SIESTA. Unstable structures having negative binding energies are sorted out. Employing the resulting relaxed coordinates we computed positron annihilation (PAS) parameters and XAFS spectra using the codes DOPPLER and FEFF-8, respectively. These data are finally compared with experimental PAS results obtained in Bonn and XAFS spectra measured at BESSY in Berlin. We will present our suggested structures of early precipitates in AlMgCu alloys and introduce the relevant methods.

[1] Y. Bagaryatsky, Dokl. Akad. Nauk CCCP 1952, Tom 87 No. 4 559-562

MM 20.9 Tue 14:45 P4

**Concerning the superstructure of rare earth compounds $RE_2PdSi_3$** — Julia Dshemuchadse, •Tilmann Leisegang, Robert Mietrach, Matthias Zschornak, Torsten Weissbach, Thomas Führlich, and Dirk C. Meyer — Nachwuchsgruppe Nanostrukturphysik, Institut für Strukturphysik, Technische Universität Dresden, Germany

A commensurately modulated structure of the series of compounds $RE_2PdSi_3$ ($RE$ = rare earth element) is presented. Accordingly, palladium and silicon atoms exhibit partial ordering on the shared B site of the $AlB_2$-type basic structure. The superstructure has been extensively studied by means of X-ray diffraction on single crystals and other X-ray techniques. Calculations based on density functional theory are compared with the found structure to clarify remaining disorder on atomic sites of the introduced model. Additionally, X-ray absorption spectroscopy measurements reveal the short-range order of $RE$ and palladium atoms, which is associated with the periodic structure. The impact of absorption on the single crystal diffraction data is analyzed by investigating randomly and spherically shaped single crystals. Using X-ray powder diffraction, a significant part of the $RE_2PdSi_3$ series is investigated to verify the model's applicability to the whole family of rare earth compounds.

We thank the DFG for financial support within the SFB 463.

MM 20.10 Tue 14:45 P4

**X-ray Diffraction Analysis and Metal Physics Modeling of Static Strain Aging and Thermal Dislocation Recovery in the Mechanically Affected Zone of Surface Finished Hardened Steel** — •Jürgen Gegner — SKF GmbH, Dept. of Material Physics, Ernst-Sachs-Strasse 5, 97424 Schweinfurt, Germany

After heat treatment, finish machining of the hardened steel represents the last manufacturing step of machine elements. The practically most important operation of grinding is applied to achieve edge zone compressive residual stresses, best surface quality and dimensional accuracy. Metal removal involves high plastic deformation work. Glide and intersection processes raise the density and produce lower energy substructures of dislocations. The temperature and time behavior of post-machining thermal treatment is analyzed on ground and honed martensitic SAE 52100 rolling bearing steel. Microstructure stabilization is reflected in a large XRD line width decrease on the surface. The kinetics is modeled by rate-controlling carbide dissolution as the carbon source for Cottrell-type segregation at dislocations. This static strain aging is verified by the formation of a slight white etching surface layer. The metal physics model is extended to also consider superimposed thermal dislocation recovery. Both effects are separable. In rolling contact fatigue tests under mixed friction running conditions, air reheating of the samples below the tempering temperature, which avoids hardness loss, leads to a significant lifetime increase. Thermal post-treatment after cold working results in similar changes of the XRD line width in the larger mechanically affected edge zone.

MM 20.11 Tue 14:45 P4

**Investigation of structure dependent resonances in split-ring resonators by terahertz time-domain spectroscopy** — •Stefan Waselikowski, Markus Walther, and Hanspeter Helm — Department of Molecular and Optical Physics, University of Freiburg

Recently metamaterials based on split-ring resonator structures raised considerable interest due to their unprecedented electromagnetic properties [1]. Their behavior is mainly dictated by the interaction of their building blocks with an incident light wave and the associated formation of electric and magnetic resonances. We use terahertz time-domain spectroscopy (THz-TDS) [2] to measure the characteristic resonances in different arrangements of metallic split-ring resonators. By varying the resonator geometry we are able to study both, the structure-dependence of the resonances as well as coupling between individual resonators. Our approach takes advantage of the ability of THz-TDS to measure amplitude and phase of the electric field over a wide spectral bandwidth. Furthermore, due to the relatively large wavelength (1 THz corresponds to $\lambda$=300 $\mu$m) structures with dimensions on the order of the wavelength can easily be manufactured by standard micro-fabrication techniques.

[1] D. R. Smith, J. B. Pendry, and M. C. K. Wiltshire, Science 305, 788 (2004)
[2] D. Grischkowsky, S. Keiding, M. Vanexter, and C. Fattinger, J. Opt. Soc. Am. B 7, 2006 (1990)

MM 20.12 Tue 14:45 P4

**Computational Study of Effective Viscosity using a coupled phase-field and Lattice Boltzmann model** — •Ali Aksi, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe, Germany

We use a coupled phase-field and Lattice Boltzmann model to measure the effective viscosity of a fluid containing a distribution of particles. The particles are defined as regions with energy bearing boundaries that may differ in their physical states. A Lattice-Boltzmann method is used to describe the motion of the particles in a flow field. We present 2D and 3D simulation results for different types of domains with different amounts of particles, distributions and volume fractions. We also show simulation results using a compressible and incompressible Lattice Boltzmann model in comparison.

MM 20.13 Tue 14:45 P4

**Materials science and reverse bioengineering - Status and potential Applications of the nanofocus endstation of $\mu$SAXS-beamline at Petra III** — •Christina Krywka[1], Stephan Roth[2], and Martin Müller[3] — [1]Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, D-24098 Kiel — [2]DESY, Notkestraße 85, D-22063 Hamburg — [3]GKSS Forschungszentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht

The new synchrotron Petra III is going be a high-brillance synchrotron radiation source, located on the site of DESY in Hamburg, Germany. For this purpose, the existing Petra storage ring is being refurbished into one of the most brillant x-ray sources worldwide and its completion is scheduled for 2009. The $\mu$SAXS-beamline of Petra III will be equipped with an additional endstation, designated to provide a high flux x-ray beam focused to about 100nm × 100nm. At the nanofocus endstation experiments with a superior spatial resolution will become available with a flux sufficiently high to study both biological and synthetic materials. This contribution presents an overview on the beamline extension and the current status of its completion. Also, exemplary and potential applications of nanofocused x-rays are shown. Among these are diffraction methods used for the structure determination of synthetic materials (e.g. metallurgy, surface science, semiconductor technology) and biological materials with multiple levels of structural

hierarchy (e.g. wood, fibres, cells).

MM 20.14 Tue 14:45 P4

**Utilization of thermodynamic databases for phasefield-simulations** — •Sebastian Schulz, Abhik Choudhury, and Britta Nestler — Institute of Computational Engineering, Karlsruhe, Germany

To get significant results out of phasefield-simulations, precise thermodynamic properties of the system to be investigated are required as input values. Those values often have to be read out of phase diagrams and typed into the input file manually. An alternative would be the automatic access on thermodynamic databases and their utilization with the Calphad method. In this contribution we intend to present a coupling of thermodynamic databases to the PACE 3D simulation software and the thereby achieved results from simulations of the aluminium/copper system.

MM 20.15 Tue 14:45 P4

**3D Polycrystalline grain structures under the influence of elastic forces** — Mathias Reichardt, •Marcus Jainta, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Germany

To predict the failure and strength properties of metallic alloys, it is neccessary to take in account the behaviour of such material under the influence of elastic forces. When applying a sufficient amount of stress, the grain structure breaks and forms a crack. In numerical simulations, we investigate crack propagation in polycrystalline metallic alloys for mode I and III. The shape of such cracks depends on the applied loads and on the grain distribution of the observed material. Suitable simulations require many grains in a relatively large domain. To achieve this goal, we present a parallel, optimized multi phase field model featuring efficient modelling of large three dimensional phase systems coupled with a model for elastic stresses. We show results for 2D and 3D crack developments along grain boundaries and in polycrystalline systems.

MM 20.16 Tue 14:45 P4

**From DFT to TB: A reliable derivation of tight-binding parameters for hard materials** — •Martin Reese[1,2], Matous Mrovec[1,2], Bernd Meyer[3], and Christian Elsässer[2] — [1]IZBS, Universität Karlsruhe — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [3]ICMM, Universität Erlangen-Nürnberg

Hard materials play an important role in industrial applications as protective coatings of tools. Recent experiments indicate that nanostructered composites of crystalline and amorphous carbides and nitrides can yield materials that reach the limit of super-hardness. However, a scientific understanding of these complex materials is still incomplete.

In the course of developing a multi-scale modelling framework for simulations of nanocrystalline transition metal carbides and nitrides we apply accurate first-principles calculations, based on the density functional theory (DFT), to derive reliable non-orthogonal and orthogonal tight-binding (TB) Hamiltonians. The TB Hamiltonians are constructed by projecting the self-consistent electronic wave functions from DFT onto a minimum basis set of atomic orbitals. This well defined procedure enables to overcome the ad-hoc fitting of TB models and presents a rigorous coarse-graining tool, which can be applied in various bonding environments. In this contribution we will present the application of the method to several model materials, namely the covalently bonded elements carbon and silicon, the transition metal titanium, and binary compounds of these elements. We will discuss the variation of the Hamiltonian matrix elements as a function of the interatomic distance and their transferability in various environments.

MM 20.17 Tue 14:45 P4

**Modelling particulate self-healing materials and application to uni-axial compression** — •Olaf Herbst[1,2], Akke Suiker[1], and Stefan Luding[2] — [1]Aerospace Engineering, TU Delft, Kluyverweg 1, 2629 HS Delft, The Netherlands — [2]2Multi Scale Mechanics, TS, CTW, UTwente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Using an advanced history dependent contact model for DEM simulations, including elasto-plasticity, viscosity, adhesion, and friction, pressure-sintered tablets are formed from primary particles. These tablets are subjected to uni-axial compression until and beyond failure displaying peak strength. For fast and slow deformation we observe ductile-like and brittle softening, respectively.

We propose a model for local self-healing that allows damage to heal during the loading process such that the material strength of the sample increases and failure/softening is delayed to larger strain. Local healing is achieved by increasing the (attractive) contact adhesion forces for those particles involved in a potentially breaking contact.

We examine the dependence of the strength of the material on (a) the damage detection sensitivity, (b) the damage detection rate, and (c) the (increased) adhesion between healed contacts. The material strength is enhanced, i.e. the material fails at larger strains and reaches larger maximal stress values, when any of the parameters (a) – (c) is increased.

MM 20.18 Tue 14:45 P4

**The relationship between the sinter-atmosphere and the phase modification of $TiO_2$ at high temperatures** — •Nicole Pfeiffer, Abdelilah Lahmar, Salah Habouti, Matthias Dietze, Claus-Henning Solterbeck, and Mohammed Es-Souni — Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany

In this work we generated $TiO_2$-nano particles on Si-substrate by solution deposition from a precursor. The films were treated under different atmospheres at ∼800°C to control the phase formation. It is shown by means of Raman scattering that anatase polymorph forms preferentially in reducing atmosphere, instead of the thermodynamically stable rutile phase. The results are discussed in terms of specific defect structures that could form in the anatase phase.

MM 20.19 Tue 14:45 P4

**Performance analysis of a parallel simulator for phase-field models** — •Alexander Vondrous, Michael Selzer, Britta Nestler, and Marcus Jainta — Institute of Computational Engineering (ICE), Karlsruhe, Germany

Parallel algorithms for the numerical solution of phase field models are used to improve calculation times. To simulate a large section of a complex microstructure and to consider effects such as fluid flow on the morphology evolution, large computational domains have to be considered. In such cases parallelization is needed to significantly increase the speed of the computation. To classify the performance of parallel computations, infomation about the used hardware is important. Performance characteristics are, among others, the speedup and the efficiency. The results of the presented performance analysis are used to optimize parallel algorithms and hardware utilization. The numerical scheme avoids calculations in bulk phase regions of the domain leading to an inhomogeneous load balance and an undesirable higher idle time of some of the CPUs in the network. To minimize this effect, dynamic domain decomposition during run time is applied. Simulations of dendritic growth in a flow field serve to evaluate the performance for different numbers of CPUs.

MM 20.20 Tue 14:45 P4

**Polarization dependent Raman spectroscopy of $LiBH_4$ single crystals** — •Britta Willenberg, Florian Gebert, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, 38106 Braunschweig, Germany

In a previous paper [1] we have reported an extensive low temperature Raman scattering study on $LiBH_4$ and $LiBD_4$ powders. The 27 observed lines have been assigned to phonon modes within the orthorhombic Pnma structure by comparing the experimental values to density functional theory (DFT) values [1]. In the present contribution we present for the first time Raman scattering measurements on small $LiBH_4$ single crystals. These have been identified among the grains of the powders (Alpha Aesar) by searching for large polarization dependencies of the Raman lines. On the basis of these new results a few of the former assignments have to be revised. Among the external modes this concerns the mode near 307 $cm^{-1}$ which is definitely of $A_g$ symmetry and not of $B_{2g}$ symmetry as had been concluded on purely energy arguments.

A second issue is the phase transition to a hexagonal structure at about 380 K. Several grains of our powder samples did not show the anticipated changes of the Raman spectra. We have now succeeded in finding a few grains which, indeed, display the characteristic simplification of the Raman spectra when the phase transition to the hexagonal phase occurs.

[1] A.-M. Racu et al., J. Phys. Chem. A 112, 9716 (2008)

MM 20.21 Tue 14:45 P4

**Low temperature Raman spectroscopy of $Mg(BH_4)_2$ and $Mg(BD_4)_2$** — •Florian Gebert[1], Britta Willenberg[1], Joachim

Schoenes[1], Michiel van Setten[2], Christoph Frommen[2], and Maximilian Fichtner[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany

We report a micro-Raman scattering study on fine powders of $Mg(BH_4)_2$ and $Mg(BD_4)_2$ for temperatures ranging from approximately 5K to room temperature. At the lowest temperature, we observe 25 lines in both compounds, which were assigned within the 86 Raman active modes, for the I-4m2 structure, whose energies have been derived using first principle calculations based on density functional theory. This structure was claimed by Ozolins et al. [1] to posses an even lower ground state energy than the $P6_1$ structure reported formerly for the low temperature $\alpha$-phase [2,3]. The comparison of theoretical and experimental values leads to straight lines with slopes between 0.98 and 1.03 for the external, bending and stretching modes, which is better than expected. Nevertheless, one can not definitively conclude that the structure is I-4m2 since a substantial number of possible lines have not been observed. This is even more so for the $P6_1$ structure. Further progress will require measurements on single crystals and/or intensity computations. [1] V. Ozolins et al., Phys. Rev. Lett. 100, 135501 (2008) [2] R. Cerný et al., Angew. Chem. Int. Ed. 46, 5765 (2007) [3] J.-H. Her et al. , J. Acta Cryst. B63, 561 (2007)