a different conditions and studied by X-ray diffraction.

The $(Na_{0.5}La_{0.5})MoO_4$ with $|\Delta r_{(Na-La)}|=r_{Na}-r_R=0.02$Å (r-ionic radius) has the scheelite structure (sp. gr. $I4_1/a$), in contrast to the $(Na_{0.5}Gd_{0.5})WO_4$ ($|\Delta r_{(Na-Gd)}|=0.13$Å) and (Na,Gd,Yb)$WO_4$ ($r_{Na}>r_{Gd}>r_{Yb}$) with the pseudo-tetragonal superstructure unit cell with double parameters. The non-annealed (growth in Ar) and annealed by 1000ºC for 4 days in air crystals of $(Na_{0.500}La_{0.445}Ce_{0.05}Er_{0.005})MoO_4$ nominal composition have "enantiomorphic" structures. The annealed by 1000ºC for 24 h in air crystal of $(Na_{0.500}La_{0.295}Ce_{0.20}Er_{0.005})MoO_4$ has the scheelite structure. A statistical distribution of oxygen on two sites of structure of non-annealed (growth in $99\%N_2+1\%O_2$) and annealed by 700ºC for 100 h in air of these crystals was found.

Keywords: sheelite, structure, properties

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Lattice Parameters Measurements of $YBa_2Cu_3O_{7-\delta}$ Superconductors Prepared under Various Forming Pressures using X-ray Diffraction Technique

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The effect of pressure on the critical temperature T_c is studied for $YBa_2Cu_3O_{7-\delta}$ compounds prepared under various forming pressures. A systematic decrease in lattice parameters is observed with forming pressure. Resistivity measurements show an increase of the onset temperature T_{cO} with forming pressure. A value of $dT_{cO}/dP\approx(0.070\pm0.010)\times10^{-8}$ K/Pa is determined. A new mechanism based on the variation of the interlayer tunneling integral $t_\perp$ is used to analyse the experiment results.

Keywords: superconductors, lattice, parameters

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On a New Wave Type Generated in Deforming Metal Crystals

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Quasi-static deformation was studied on tensile fcc, bcc and hcp single crystals by holographic technique. It iahs been found that slow wave processes are generated in the deforming material. These involve concerted motion and temporal evolution of local flow nuclei whose nature is defined by micro-scale self-organization mechanisms.

The wave pattern type is determined for a given flow stage by work hardening law $\theta(\varepsilon)$, where $\theta=G^{-1}\cdot d\sigma/d\varepsilon$ is the work hardening coefficient; G, the shear modulus; σ, the plastic flow stress and ε, the deformation. The waves are characterized by wavelength $5\leq\lambda\leq10$mm propagation rate $10^{-5}\leq V\leq10^{-4}$m/s and frequency $10^{-3}\leq\omega\leq10^{-2}$Hz. The waves are found to exhibit the following regular features: wave rate $V=\Xi/\theta$, where $\Xi=const\approx10^{-7}$m/s; quadratic dispersion law $\omega(k)=1+k^2$ and a concurrent decreases in the entropy of material by wave generation $\Delta S<0$.

These can be likened to quasi-particles whose mass as calculated from the de Broglie equation for all the monocrystals tested $m=h/V\approx1.5$amu and dimensionless mass $\mu=m/A$ (A is the respective metal's atomic mass) are found to grow with the number of electrons n per metal unit cell as $\mu=\mu_0+\kappa n$.

Thus it is contended that by plastic flow slow waves would be generated spontaneously in a single metallic crystal, which is regarded as a complex thermodynamically open system. The nature of these wave processes and their role on plastic deformation are discussed.

Keywords: plasticity, wavelength, entropy

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Structure and Magnetic Properties of 3-substituted-5-(2-pyridyl) Pyrazole Metal(II) Complexes

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Five substituted pyridyl-pyrazole metal(II) complexes, [Fe(Hpp-*But*)$_3$(*X*)$_2$], *X*=ClO_4^- (***1***), BF_4^- (***2***), [Co(Hpp-*But*)$_3$(ClO$_4$)$_2$] (***3***), *cis*-[Fe(Hpp-ϕ)$_2$(NCS)$_2$] (***4***) and *trans*-[Fe(Hpp-ϕ)$_2$(NCS)$_2$]·(H$_2$O)$_2$ (***5***), were synthesized. Molecular and crystal structures of these complexes were investigated by single crystal structure analysis. The comparison in molecular structures between these complexes will be presented. The magnetic properties were studied by SQUID magnetometer.

Complex (***1***) and (***2***), with t-Butyl substituted group, are spin-crossover compounds. Complex (***1***) is a gradual but completed spin transition from RT to 200K. The Fe $L_{2,3}$-edge of iron(II) of (***1***) and (***2***) X-ray absorption spectroscopy are studied using synchrotron radiation. The apparent change due to HS-LS transition will be presented in coordination geometry around Fe and in Fe core electron excitation. However, compound (***4***) and (***5***), with substituted phenyl group, show no spin transition phenomenon within the temperature range studied. The relationship between structure and magnetic properties will be discussed.

Keywords: structure-magnetism relationships, spin crossover, magnetism

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X-ray Absorption Studies of Fe-btr Spin Crossover Complexes

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The aim of this work is to take the advantage of the X-ray absorption spectroscopy to get insight into the evolution of electronic configuration in HS and LS states of the specific absorption atoms at various temperatures and also in the LIESST state. Three Fe spin crossover complexes, (**1**) Fe(btr)$_2$(NCS)$_2$·H$_2$O[1], (**2**) Fe(btr)$_3$(ClO$_4$)$_2$[2] and a Co doped Fe_xCo_{1-x}(btr)$_2$(NCS)$_2$·H$_2$O[3] (**3**) were chosen to be studied. With temperature changing **1** shows an abrupt spin transition with a hysteresis of 25K ($T_{1/2}\downarrow$ = 119.8K and $T_{1/2}\uparrow$ = 145.1K) while **2** was found to behave as a two-step spin crossover complex.

K-edge absorption spectra of **1** and **3** were collected in both RT (HS) and 16K (LS) and also after irradiating by a laser light of 532 nm. The existence of the HS-2 after irradiation in both **1** and **3** is varified by Fe K-edge spectra. However, spin transition only occurs at Fe site not at Co site, though they should be situated on the same site.

Fe L-edge spectra of **2** illustrate a two-step spin transition; one is abrupt and the other one is gradual, which is consistent with the results reported earlier.

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Keywords: spin-crossover, X-ray absorption, Fe(II) complexes

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Change of Structure and Properties of System WC-Ti at Mechanical Activation

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Tungsten carbide is one of the most interesting representatives carbides transition of metals of maximum groups, which can have as cubic, and hexagonal crystallographic modification. In particular, cubic WC with structure as NaCl has rather wide area homogeneity on carbon and has high temperature melting, hardness and durability, and also propensity to formation double carbides with transitive 3d-metals. The data about peculiarities of the chemical bonding and changes in then electronic structure of the cubic WC at partial replacement of