covering, for example, the utilisation and protection of ground water, the foundations of skyscrapers, the sealing of waste deposits, canalisation systems, railway and road construction, and the redevelopment of waterways and the soil. The determination of the crystal structure of senaite has progressed to the point where a trial model consisting of all atoms has been defined. Plumboferrite has been examined and found to have the magnetoplumbite substructure. The structure of CoGeO3 has been refined in detail and the occurrence of polytypism in this compound is readily explained by the approximation to closest packing.
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Keywords: General Geoscience, Inorganic crystallography, Geosciences

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Thickness dependent crystallographic transition in Fe/Ni superlattices

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The 3d transition metals have historically got a huge attention due to both interesting physical properties as well as the applications of systems containing such elements. FeNi alloys, in all concentration ranges, are of particular interest due to industrial applications with emphasis on the so called Invar [1]. While body centered cubic (bcc) Fe is ferromagnetic at room temperature, face centered cubic (fcc) Fe can posses rich variety of magnetic phases. Mossbauer spectroscopy, due to its sensitivity to magnetic and structural environment, is a powerful technique for studying such systems and also because it can isolate Fe magnetism. In contrast to previous studies, where a thick Ni layer has been used as buffer layer and then a thin Fe layer has been establish as fcc structure on that, here another approach has been tried. By starting with higher thickness of Fe than Ni, a bcc structure is established. By increasing the Ni thickness, the structure should transit gradually from bcc to fcc. This transition is however smooth, i.e. there will be coexistence of both faces. Several sample series of Fe/Ni superlattices with varied x ML of Fe and y ML of Ni were grown by dc magnetron sputtering method onto MgO substrate. In the first sample series the ratio x/y was kept constant, while the bilayer thickness was changed. In the second sample series, the ratio x/y was also changed. The study of the first series showed that the bcc structure persisted and was almost insensitive to changes of the interface density. The result from the study of the second sample series, where the ratio x/y was changed, i.e. thickness of the Ni layer increased while the thickness of Fe layer was unchanged, showed a gradual transition from bcc to fcc.
[1] B. Window, J. Appl. Phys. 44 (1973) 2853.

Keywords: Mossbauer Spectroscopy, Fe/Ni Superlattices, Magnetism

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Combined use of crystallography and mass spectrometry for ligand characterization and drug design

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AliX has developed FAMASS (Fragment Analysis by MASs Spectrometry), a proprietary approach for structure-based drug discovery combining X-ray crystallography and non-covalent mass spectrometry. We routinely use non-covalent electrospray ionization mass spectrometry to check the purity and the functionality of proteins used in [protein-ligand] complex crystallization, and also to screen ligands for binding to given targets. This is especially interesting when a functional assay is not available, as in the case of orphan nuclear receptors. Non-covalent mass spectrometry is an efficient secondary screening method to discard false positives from a high-throughput primary screening. We have now extended this approach to fragment-based drug discovery. Fragments selected by in silico screening are validated for physical binding to the target by non-covalent mass spectrometry. Validated fragments are then co-crystallized with the target and their mode of binding elucidated by crystallography, paving the way toward the design of new scaffolds.

Keywords: protein-ligand complex, mass spectrometry, fragment-based drug discovery

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Teaching how to simply replace the independent atom model - the example of Bergenin

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In four years the crystallographic community will celebrate 100 years of X-ray diffraction. While in the first 50 years the method was applicable only in exceptional cases, the developments in the second half of the last century increased the number of published X-ray structures dramatically, so that the number of CCDC entries is quickly approaching half a million. Nevertheless, in almost all cases the independent atom model (IAM) was applied that uses spherical scattering factors which do not allow a proper description of chemical bonding. To replace the IAM with an aspherical scattering model we recently introduced the concept of Invarioms, generated an Invariom library and corresponding software for a straightforward application [1]. Since the needed X-ray and computer equipment is far from expensive up-to-date standard and since we will show that the use of the Invariom model can easily be taught, the aspherical Invariom model is best suited to be used by groups also in less developed countries. This is demonstrated by the example of Bergenin, a compound of traditional Asian medicine, which is known for anti-HIV and other biological activities. On a more than 20 years old diffractometer a low resolution (sin(theta)/lambda= 0.60 A-1) data set was measured at room temperature that was properly suited to obtain an improved molecular geometry compared to the IAM and a variety