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Structural modulation in ferromagnetic shape memory martensitic phases. Lara Righi. *Dipartimento di Chimica GIAF, Università degli Studi di Parma, Parma, Italy.*
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Multifunctional ferromagnetic shape memory Heusler Ni-Mn-Ga alloys are frequently characterized by structural modulation in martensitic phases. In particular, modulated martensitic phases, showing the higher magnetic field induced strain performance, are the most promising candidates for technological applications. Depending on the composition, as well as pressure and temperature conditions, this periodic structural distortion, consisting of shuffling of atomic layers along defined crystallographic directions, accompanies the martensitic transformation. Over the years, different Ni-Mn-Ga modulated martensitic structures have been observed and classified depending upon the periodicity of corresponding ideal *n*M superstructure (where *n* indicates the number of basic unit cells constituting the superlattices). On the other hand, it has been demonstrated that in most cases such structural modulation is incommensurate and the crystal structure has been fully determined by applying superspace formalism [1,2]. The results, obtained by structure refinements on powder diffraction data, suggest a unified crystallographic description of the modulated martensitic structures, here presented, where every different "*n*M" periodicity can be straightforwardly represented.

[1] Righi L., Albertini F., Calestani G., Pareti L., Paoluzi A., Ritter C., Algarabel P.A., Morellon L., Ibarra M. R.. *J. Solid State Chem.* 2006, 179, 3525. [2] Righi L., Albertini F.,Villa E., Paoluzi A.,Calestani G., V. Chernenko V., S. Besseghini S., C. Ritter C., F. Passaretti F., *Acta Mater.* 2008, 56, 4529.

Keywords: shape-memory alloys, martensitic alloys, incommensurate modulated structures

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Simulation of modulated reflections. Jeffrey J. Lovelace[a], Martyn D. Winn[b], Gloria E. O. Borgstahl[a]. [a]*The Eppley Institute for Research in Cancer and Allied Diseases, USA.* [b]*Computational Science and Engineering Department, STFC Daresbury Laboratory,UK.*
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In a modulated crystal, the repeating unit is not periodic but contains a disorder of the molecules that can sometimes be described with a mathematical function. In the diffraction pattern from such a modulated crystal the standard periodic main reflections are flanked by satellite reflections. Generally, incommensurately modulated crystal diffraction cannot be simply described using integers along the reciprocal-lattice directions. However, in the special commensurate case where the satellite spacing is rational relative to the main reflections, a supercell can be used to describe the modulation. Using a supercell allows structural processing to proceed in a 'normal' fashion but with the downside of dealing with many more atoms. Not much is known about the relationship between a highly modulated macromolecular crystal and the resulting satellite intensities so in this study a modulated protein crystal was simulated using a supercell approach. The protein superstructure was modulated to varying degrees and the resultant diffraction patterns and electron-density maps were studied to understand better how a modulation may manifest itself in real protein data. In the case that was evaluated, relatively small structural modulation resulted in significant satellite intensities. Interesting cases were observed where extinguished main reflections had strong satellites.

Keywords: incommensurate crystallography, modulated protein crystals, computer simulation

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Formation and stability of quasicrystals and other complex intermetallics. Walter Steurer. *Laboratory of Crystallography, ETH Zurich, Switzerland.*
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Already the early rapid solidification experiments on Al-Mn showed that quasicrystals (QC) can grow much faster than their approximants. This has been mainly attributed to the lower nucleation barrier of QC due to the local icosahedral order already present in the melt. However, this does not explain, how quasiperiodic long-range order can be established without much diffusion and why never high rational aproximants are formed instead. What lets quasiperiodicity win over the periodic order of approximants? Certainly not the perfect regularity of icosaheral clusters that is possible in QC. The fundamental clusters are in both cases equally distorted, they are far from ideal icosahedral symmetry. Another open question is why the structures of QC are closer to ideal quasi-periodicity than to the averaged one of random tilings.
I will present models that offer answers to some of these questions. Beside other factors, particularly the role of clusters and flat atomic layers for the growth and stability of QC and other complex intermetallics will be discussed. An example is illustrated in Fig. 1, where the projected structures of an icosahedral QC, its 1/1-approximant and the largest known intermetallic structure are shown. It is obvious that all atoms of the QC are located on quaisperiodically spaced sets of flat atomic layers which obey the icosahedral symmetry. A completely different picture is obtained along the pseudo-5-fold direction of the 1/1-approximant although the local structures are similar. I this case the icosahedral symmetry of the clusters does no more coincide with the symmetry of the cubic approximant. It is also remarkable that all structures of intermetallics with periodic structures and giant unit cells show an analogue abundance of flat atomic layers what is already well known for Frank-Kasper phases. The interplay of cluster formation in a framework of atomic layers assists atoms to find their sites in unit cells with thousands of atoms.

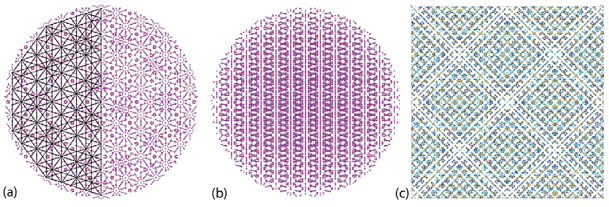

Fig. 1 Projections of the structures of (a) *i*-$Cd_{84}Yb_{16}$ along the 5-fold axis, (b) 1/1-Cd_6Yb along the pseudo-5-fold axis and (c) *cF*(23,256-*x*)-$Al_{55.4}Cu_{5.4}Ta_{39.1}$ along [100].