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The importance of characterizing incommensurately modulated structures for the study of physical properties

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Abstract

The presentation focuses on the practical significance of the results of the study of different incommensurable modulated structures. Details of these studies can be found in the cited publications.

Layered transition metal dichalcogenides are usually classified as materials with quasi-two-dimensional metallic conductivity appearing in layered planes. It was shown that this rule does not hold for 1T-TaS_2, where the in-plane temperature (pressure) dependent conductivity is not metallic, whereas the out-of-plain one is metallic [1]. This phenomenon was explained on the basis of determining the incommensurately modulated crystal structures of 1T-TaS_2 at different temperatures and pressures [1].

The effect of the incommensurately modulated structure of iron-deficient $Fe_{1.35}Ge$ on the temperature dependence of its resistivity shows that a large number of ordered Fe-vacancies introduce strong backscattering similar to disordered structures. The $Fe_{1.35}Ge$ system is on the verge of the Mooij correlation [2]. A similar effect resulting in saturated metal resistivity is also observed for the $Sr_2Pt_{8-x}As$ incommensurately modulated structure [3].

The luminescence properties of $Na_xEu_{3+(2-x)/3}MoO_4$ scheelite-like structures were shown as a function of Eu- dimers occurring in their incommensurately modulated structure [4].

$Ba_4Fe_4ClO_{9.5-x}$ crystals, are interesting cases of tunable structure modulations [5]. The exact properties of these newly obtained compounds have not yet been studied, but they seem very promising.

The importance of methylammonium lead iodide, $MAPbI_3$, for solar cell development is well established. However, the properties of this compound are very sensitive to a phase transition around 330 K, which is expected to occur at the operating temperature of this compound. Cycling the compound around this temperature shows stabilization of an incommensurately modulated structure [6], which reduces the efficiency factor. This knowledge will allow appropriate operational adjustments to be made.

References

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Sketch of the MAPbI3 transformation during cycling