Physicists supervise the formation of higher manganese silicide films

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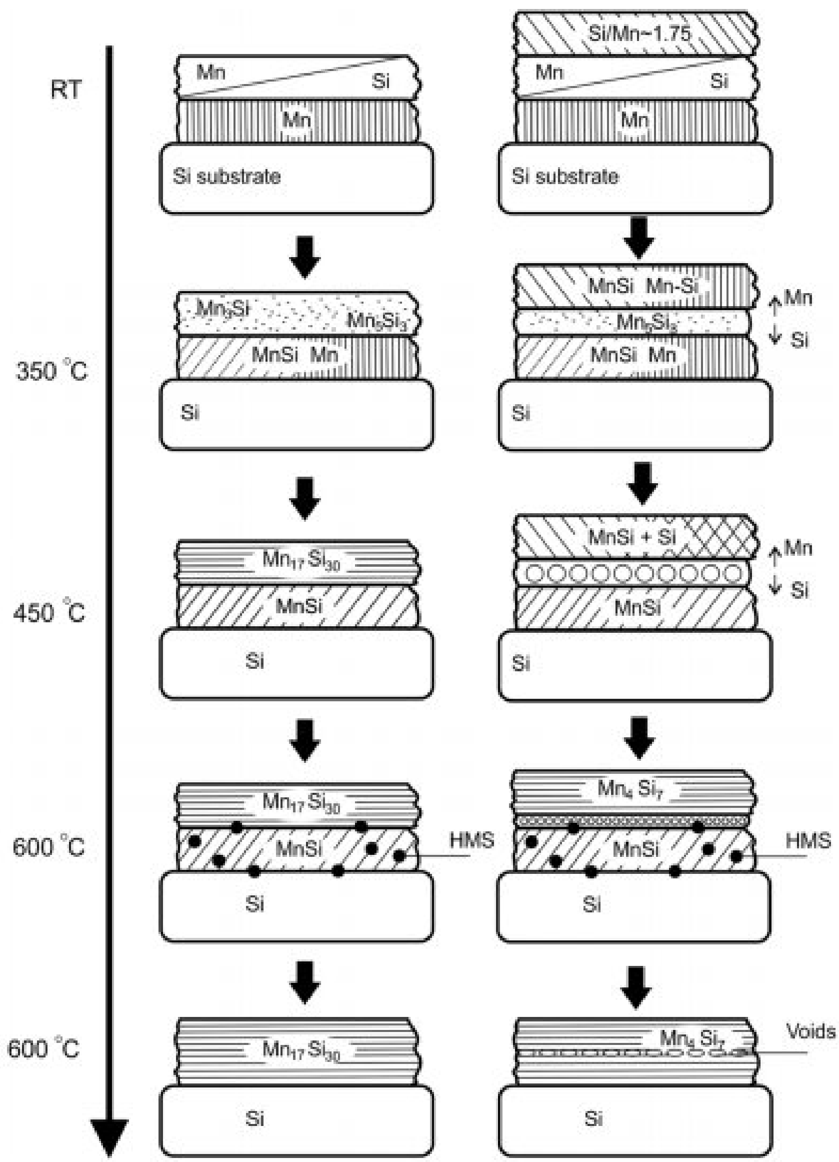

Schematic illustration of the synthesis procedure for left: Mn17Si30 and right

Mn4Si7 sample. Credit: Ivan Tarasov

A team from Kirensky Institute of Physics (Siberian Branch of the Russian Academy of Sciences) together with colleagues from Siberian Federal University have offered an approach for the controlled synthesis of semiconducting higher manganese silicide thin films. The films may be used in thermoelectric converters and other devices. The team also suggested other areas of application for these materials. The results of the work were published in *Journal of Materials Science*.

Higher manganese silicides (MnSi~1.75) are a group of manganese and silicon compounds with an exotic crystal structure called "chimney-ladder." Manganese atoms form the chimney itself, and silicon is shaped similar to helices. Compounds attributed to this group differ from each other by the twist of helices. In Mn_4Si_7, the most famous member of the group, manganese is less twisted than in the other 11 phases known. Still, the twist maximum of helices in such a structure is unknown, as well as the means of targeted synthesis of a particular structure belonging to the group.

There is also an ambiguity in their physical properties. To carry out the targeted synthesis of different phases of higher manganese silicides on a silicon substrate, which may be used for thermoelectric and photovoltaic converters, optoelectronic and spintronic devices, is still rather difficult for the scientists. As a rule, to obtain higher manganese silicide thin films, manganese and silicon are placed on the silicon substrate, and afterwards, the system is annealed. In this condition, silicon atoms diffuse from the silicon substrate to the reaction zone and may change the phase formation sequence drastically as the amount of silicon in different higher manganese silicide phases varies within less than 1 percent. Due to such diffusion, it is impossible to obtain a desirable higher manganese silicide phase on silicon substrate just placing the required amount of manganese and silicon, and then heating the system. Silicon atoms from the silicon substrate change the silicon content in the film uncontrollably. The team aimed to resolve this issue during the study.

Two phases of higher manganese silicides were selected for targeted synthesis: Mn_4Si_7 with the least and $Mn_{17}Si_{30}$ with the most twisted helices. Like the majority of well-known higher manganese silicides, the first phase has p-type conduction. When the substance is heated, its covalent links are distorted, and free electrons start moving around. This creates holes that move in the direction opposite to that of the electrons. The second phase shows n-type conduction. In this case, the free electrons are the charge carriers.

"In this work, we used an unusual approach to the synthesis of samples. We assumed that if higher manganese silicides uncontrollably form from the amorphous mix, their formation from the mixtures of phases of other manganese silicides with higher manganese content shall differ as well for different phases. Whatever the elements on the silicon base, a compound from the higher manganese silicide family will always be the last stage. Having conducted some simple thermodynamic calculations, we found out what should be placed on the base for Mn_4Si_7 and $Mn_{17}Si_{30}$ phases to form," explained co-author Ivan Tarasov, a research fellow at the laboratory of the physics of magnetic phenomena, Kirensky Institute of Physics (Siberian Branch of the Russian Academy of Sciences).

The scientists decided to implement this idea and obtained the targeted structures. Afterward, their physical properties were studied as well. The n-type conductivity of $Mn_{17}Si_{30}$ was not confirmed. Theoretical calculations showed that the reason might be silicon vacancies, i.e. the absence of atoms in the places where they are expected to be in the $Mn_{17}Si_{30}$ crystal structure. The team registered the highest charge carrier mobility in higher manganese silicide films.

"After studying the properties of the new phase of higher manganese silicide we obtained quite interesting results. Most importantly, the approach we developed for synthesising such films proved to be effective. In the future, we will improve it to obtain different silicides with the properties required for use in actual thermoelectric and photovoltaic devices," concluded co-author Anton Tarasov, senior lecturer at Siberian Federal University.

Provided by Siberian Federal University