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Laser heating simulation of Au-Si composite structure

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Amorphous and microcrystalline silicon is important in electronics, energy and medicine due to its useful properties. Precisely, microcrystalline silicon is preferred for its high resistivity to degradation, electrical properties and special light absorption. However, producing high quality microcrystalline silicon is challenging. It requires precise control of process of crystallization and grain size.

Laser crystallization and metal-induced crystallization (MIC) are among the most advanced methods. The presence of metals during irradiation of the samples decreases the crystallization temperature and improve the properties of the final material.

In this work, the process of laser heating of an amorphous silicon film with and without a gold layer is modelled. The heat conduction equation is solved by the finite difference method. A finite difference scheme with a time step of 0.01~ns and a spatial step of 0.005~nm provided precise modelling results. This provides high accuracy of the obtained results.

The temperature field in the composite material and dynamics of the thickness of the modified layer are calculated. It was determined that the threshold of modification intensity in the \(\alpha\)-Si/Au/c-Si structure is 2 times lower than in \(\alpha\)-Si/c-Si and is \(4.3 \cdot 10^{11}\)~W/m\(^{2}\) and \(2.1 \cdot 10^{11}\)~W/m\(^{2}\) for a 1~ns pulse. The modification depth reaches \(10-20\)~nm at \(3.0 \cdot 10^{11}\) to \(8.0 \cdot 10^{11}\)~W/m\(^{2}\) for \(\alpha\)-Si/Au/c-Si and \(7.0 \cdot 10^{11}\) to \(2.0 \cdot 10^{12}\)~W/m\(^{2}\) for \(\alpha\)-Si/c-Si. The results are in good agreement with the experimental data.

Numerical simulation of the heating of multilayer structures allow to determine the best parameters of laser radiation necessary to achieve the crystallization threshold and further modification of the amorphous phase. The results can be used to optimise the experimental synthesis of microcrystalline silicon at different scales.

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