Energy Generation

First Solar optimizes semiconductor properties in crystalline structures

The performance of semiconductor devices such as solar cells, detectors, etc., depends strongly on the properties of materials used in their fabrication.

Deep understanding of these properties and the ability to tune them is critical for the development of new generations of advanced photovoltaics and electronics. First Solar, the world's largest manufacturer of thin-film solar panels, is using resources from the Ohio Supercomputer Center (OSC), to predict and optimize semiconductor properties in crystalline structures such as cadmium telluride (CdTe).

Although the efficiency of commercial CdTe photovoltaic material has grown dramatically in recent years, the advances in performance and stability of CdTe devices are achieved mostly through costly experimentation and process development while lacking theoretical guidance.

"Our research is aimed at theory-driven understanding and optimization of CdTe-based solar cells performance and stability for clean energy generation," said Dmitry Krasikov, development engineer at First Solar.

CdTe semiconductor, used for decades in X-ray detectors, has recently become the material of choice for the multi-gigawatt-per-year, thin-film photovoltaic industry. The semiconducting properties of CdTe is determined by the structures of pure crystals and imperfections, or defects. While the word "defects" often carries negative meaning, it is the defects in CdTe that make them useable in practical applications.

Though CdTe crystals always contain some intrinsic imperfections, engineers can intentionally introduce defects to give semiconductors unique, application-specific properties. The concentrations of defects and their positioning in the device structure define the electrical behavior of the device. These depend strongly on the process conditions, such as annealing temperatures, quenching rates and field operation conditions. Concentrations, spatial distributions and charge states of defects can change as a results of different diffusion, reaction and ionization processes. To understand and describe these processes, engineers first need to know the fundamental parameters of defects and reactions.

First Solar uses theoretical calculations of the parameters of defects and reactions, such as defect formation energy, reaction energy and energy barriers of elementary processes, to feed the models describing the formation and evolution of defect concentrations and recharge of the defects. These accurate, state-of the-art methods require considerable parallel computational resources to treat systems large enough within a reasonable time frame.

"This is why we are using OSC supercomputer resources in our work," Krasikov said.

Through First Solar's research and development, their large-scale solar farms can deliver energy to utilities at prices that are lower than fossil fuels. •

▶ Above: To date, First Solar has sold 13.5 gigawatts worth of solar panels, enough to power more than 2 million homes in the United States.

Below: First Solar's factories produce solar panels at a rate of approximately one every second.

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