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Close-ups of grain boundaries reveal how sulfur impurities make nickel brittle

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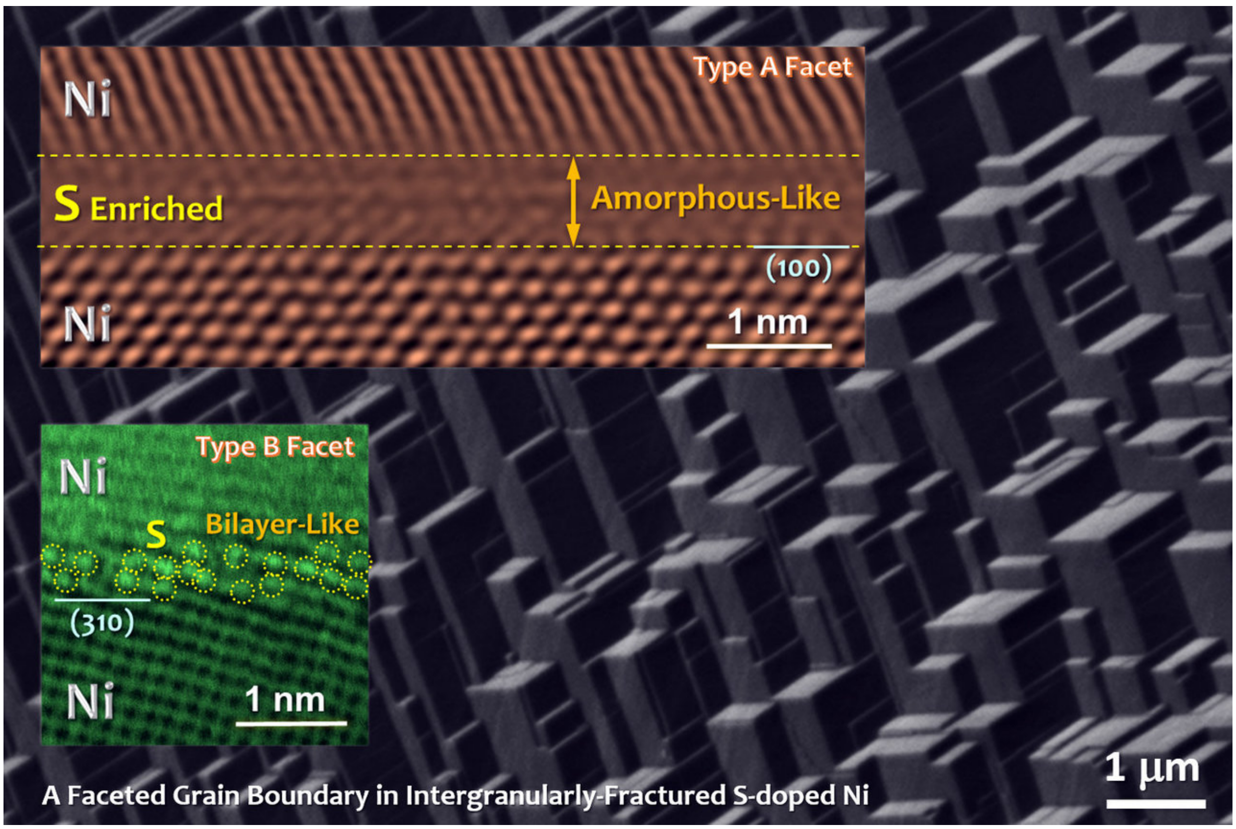

Faceted grain boundary in intergranularly-fractured sulfur-doped nickel. Credit: Jian Luo et al.

Engineers at the University of California San Diego have shed new light on a scientific mystery regarding the atomic-level mechanism of the sulfur embrittlement of nickel, a classic problem that has puzzled the scientific community for nearly a century. The discovery also enriches fundamental understanding of general grain boundaries that often control the mechanical and physical properties of polycrystalline materials.

The study was led by Jian Luo, a professor of nanoengineering and materials science and engineering at the UC San Diego Jacobs School of Engineering. The work is published July 17 in *Nature Communications*.

Since the early 1900s, engineers and scientists have recognized that sulfur impurities cause nickel and other ductile metals, such as iron and steel, to fail at low stress levels. Sulfur embrittlement of metals is of general technological importance because many engineered alloys are used in sulfur-bearing environments, such as the nickel-based high-temperature alloys used in next-generation coal-fired power plants for increasing energy efficiency.

Researchers have known that this embrittlement is related to the grain boundary segregation of sulfur, but the underlying atomic mechanisms have remained elusive.

UC San Diego engineers have shed new light on these mechanisms by examining general grain boundaries in nickel polycrystals doped by sulfur. They used a combination of aberration-corrected scanning transmission electron microscopy and semi-grand-canonical ensemble atomistic simulations.

Luo's team found that competition between interfacial ordering and disordering leads to the alternating formation of amorphous-like and bilayer-like facets at general grain boundaries. They also found that bipolar interfacial structures cause brittle intergranular fractures between polar sulfur-nickel structures that are disorderly aligned in two opposite directions.

"Similar mechanisms may cause grain boundary embrittlement in other metal-nonmetal systems. Examples include oxygen, sulfur, phosphorus and hydrogen embrittlement of other metals and alloys. These are of broad technological importance," said Luo.

This work further advances previous research by Luo's group on the bismuth embrittlement of nickel, which was done in collaboration with Lehigh University and published in two subsequent reports in *Science* in 2011 and 2017. Researchers discovered that highly-ordered interfacial structures form at general grain boundaries in bismuth-doped nickel. In the new *Nature Communications* study, Luo's group found that disordered bipolar interfacial structures form in sulfur-doped nickel.

"Bismuth and sulfur are two well-known embrittling impurities for nickel. Interestingly, we found that these represent two extreme cases of interfacial structures—ordered versus disordered, respectively. Thus, they may be considered as two classic examples of grain boundary embrittlement with different underlying atomistic structures," Luo said.

Aside from embrittlement mechanisms, researchers say this study sheds new light on the mysterious abnormal grain growth phenomena in sulfur-doped nickel, and enriches fundamental understanding of disordered interfaces. This study also challenges a traditional view by showing that the orientation of the grain boundary facet, instead of the misorientation, dictates the interfacial structure.

"This work broadens our fundamental knowledge of materials interfaces beyond the well-characterized ordered interfaces and special symmetric boundaries in artificial bicrystals that have been the focus of most prior studies. Now, we have new insight into the disordered interfaces and general grain boundaries in real-world polycrystals, which often limit the performance of most engineered materials," said Luo.

More information: Tao Hu et al, Role of disordered bipolar complexions on the sulfur embrittlement of nickel general grain boundaries, *Nature Communications* (2018). DOI: 10.1038/s41467-018-05070-2

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