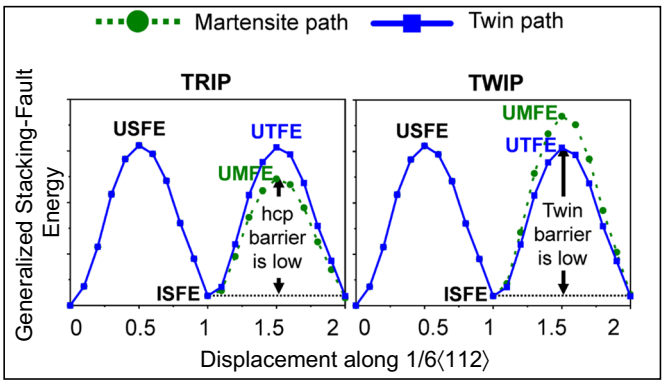
Tailored unstable fault energies accurately predict deformation in metastable high-entropy alloys

In unraveling and predicting deformation/strengthening mechanisms of high-entropy alloys (HEAs), transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP) have stood out in previous works. TRIP assesses how the strength of an alloy increases when its microstructure changes from one phase to another (in most cases, the new phase is harder). TWIP describes the increase in the strength of an alloy due to deformation by a type of microstructural/atomic readjustment. The study of TRIP/TWIP has been based on intrinsic stacking-fault energy (ISFE), an excess energy linked to the dissociation of lattice dislocations. However, it has been suggested that the ISFE approach is an inadequate metric for studying or predicting deformation in HEAs. Now, a research group from the University of Pittsburgh, the Illinois Institute of Technology, and Northwestern University have delved into this issue and reported their study in a recent issue of *Science Advances* (https://www.science.org/doi/10.1126/sciadv.abo7333). They reveal a strategy for designing metastable HEAs, and validate its effectiveness by discovering seven alloys with experimentally observed metastability for TRIP/TWIP.

In their review of past work, the researchers showed that the prediction of TRIP/TWIP formation using ISFE is unreliable, especially in HEAs. For example, $Co_{10}Cr_{10}Fe_{40}Mn_{40}$ (a TRIP alloy) was wrongly regarded as a TWIP alloy because of a low ISFE, some experiments overestimated ISFE, and density functional theory (DFT) calculations gave negative ISFE values for TRIP HEAs.

The research team, led by Wei Xiong, the director of the Physical Metallurgy and Materials Design Laboratory at the University of Pittsburgh, and Professor Wei Chen of the Department of Mechanical, Materials, and Aerospace Engineering at the Illinois Institute of Technology, applied a novel approach to this problem by considering two metrics called the "unstable martensite fault energy" (UMFE) and "unstable twin fault energy" (UTFE). UMFE represents the energy barrier associated with transformation whereas UTFE depicts the energy barrier to deformation in an alloy's atomic structure. According to the authors, "The differences between UMFE/UTFE and ISFE define the energy barrier for martensite/twin formation, which controls the competition between different deformation mechanisms and allows us to predict the TRIP/TWIP behaviors in HEAs."



Unstable martensite fault energy (UMFE) and unstable twin fault energy (UTFE) from density functional theory calculation for transformation-induced plasticity/twinning-induced plasticity (TRIP/TWIP) design. ISFE is intrinsic stacking-fault energy; hcp is hexagonal-close-packed. Image credit: *Science Advances*.

The team's data-driven alloy design employed a high-throughput Calculation of Phase Diagrams (CALPHAD) and DFT modeling. The researchers selected seven HEAs, whose face-centered-cubic (fcc) stability compares well with reference alloys $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$ (more stable fcc) and $Co_{10}Cr_{10}Fe_{40}Mn_{40}$ (less stable fcc, a candidate of fcc + hcp phases). The approach they employed considered the passage of Shockley partial dislocations through a supercell model of fcc lattice. The difference between the UTFE and ISFE was determined to be the energy barrier for twin nucleation.

The results were validated with a series of experiments and concluded that the UMFE/UTFE criterion can predict the deformation mechanism more accurately than ISFE. The researchers re-emphasized their claim that "we verified our criteria with 9 high-entropy alloys, including 7 newly designed HEAs, and 4 steels."

In a separate interview with *MRS Bulletin*, William Curtin of Brown University, who is also Professor Honoraire at the École Polytechnique Fédérale de Lausanne in Switzerland, who is not involved in this work, specified that the considered parameter is not *directly* measurable.

As a bottom line, the study showed that the UMFE/UTFE criterion provides an effective paradigm for developing metastable alloys with TRIP/TWIP for enhanced strength-ductility synergy in HEAs.

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