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Characterizing the Tensile Strength of Metastable Grain Boundaries in Silicon Carbide Using Machine Learning

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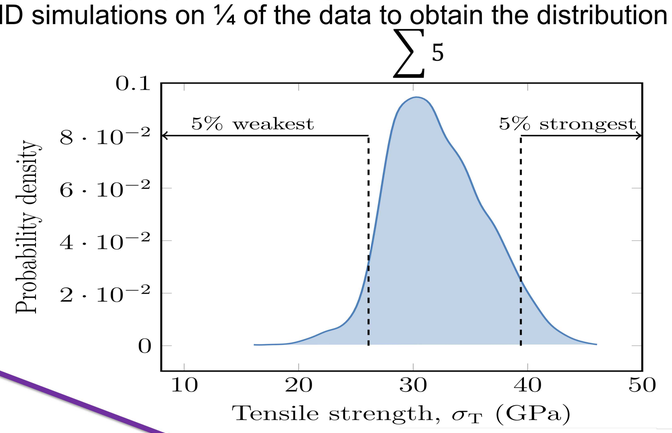
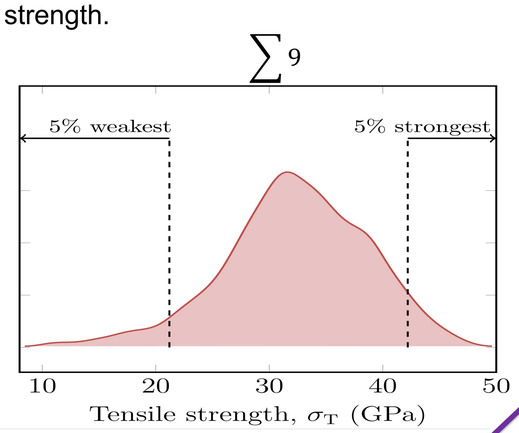
1. What Controls the Strength of Metastable Grain Boundaries?

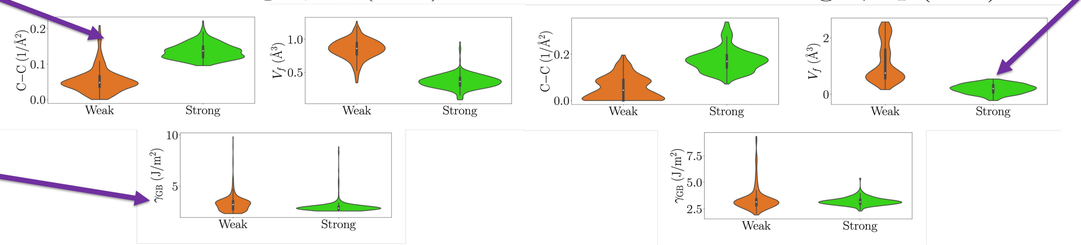
- We generated 30,000 metastable grain boundaries for the $\sum 5$ and $\sum 9$ tilt grain-boundary configuration using a computationally-efficient, Monte Carlo grain-boundary optimization algorithm[1].
- We performed MD simulations on ¼ of the data to obtain the distribution of strength.





Weak grain boundaries (5th percentile) have low amounts of C-C bonds

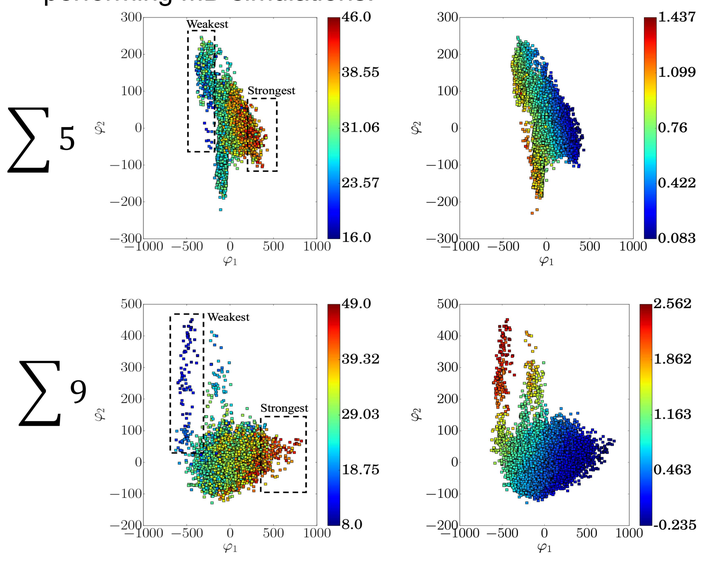
Strong grain boundaries (95th percentile) have low Excess Free Volume



Grain-boundary energy is not a good indicator of strength

2. Low-dimensional Representation of the Local Atomic Environment of Metastable Structures

- We coupled the SOAP descriptor[2] with PCA to identify weak and strong metastable grain boundaries without performing MD simulations.



Tensile Strength σ_T **Excess Free Volume V_f**

In Brief

Problem: The local atomic structure and chemistry of grain boundaries control the tensile strength of silicon carbide components (SiC). However, predictions for the properties of SiC grain boundaries are currently limited to their ground state configurations despite the fact that recent studies[1] have shown that a significant number of grain boundaries are not in the ground state.

Approach:

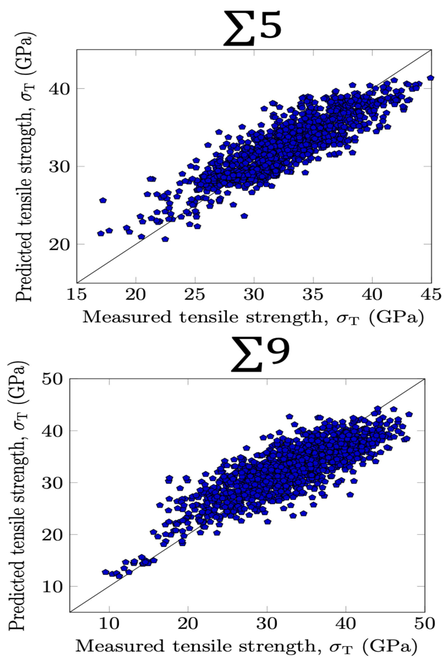
- **High-throughput atomistic simulations** to create a large set of metastable grain boundary structures and to calculate the grain boundary tensile strength strength.
- Used **16 descriptors** to describe local atomic structure and chemistry of each grain boundary.
- Used **boosted-regression trees** (BRT) to predict the metastable grain-boundary strength as a function of these descriptors.

Results:

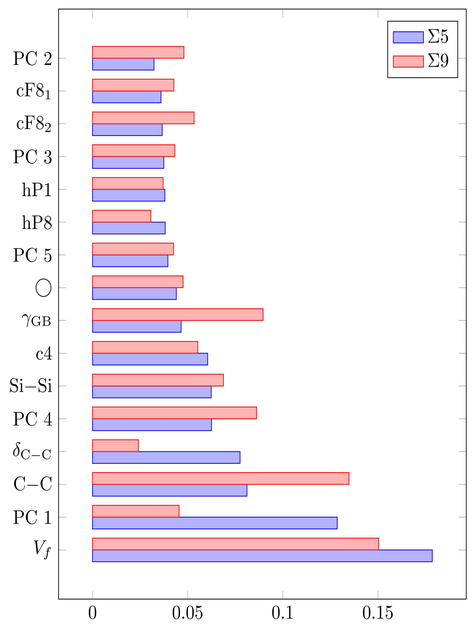
- **Rapid prediction of grain boundary tensile strength.**
  - BRT-based surrogate model accurately predict the tensile strength without the need to perform any molecular dynamics (MD) simulations .
- **Efficient identification of strong and weak grain boundaries** using a low-dimensional representation of the grain boundary structure.
- **Determination of the features that control the strength of grain boundaries:**
  - The tensile strength of a generic metastable SiC grain boundary is primarily dominated by the excess free volume and the amount of C-C bonds.
  - The 5% strongest metastable grain boundaries have high amounts of C-C bonds, low Excess Free Volume and are insensitive to the type of local structure.

3. Surrogate Model to Predict Grain Boundary Strength

- The model was trained on 80% of the data and validated on the remaining 20%.



Parity Plot of Test Dataset



Feature Importance Plot

Table of Mean Absolute Percent Errors

CSL	Training Error (%)	Average 5-fold Cross Validation Error (%)	Testing Error (%)
∑5	4.25	5.19	5.12
∑9	7.73	9.72	9.03

List of Symbols

Symbol	Description (unit)
γ_{GB}	Grain-boundary energy (J/m^2)
V_f	Grain-boundary excess free volume ($Å^3$)
C – C	Carbon-carbon bond density ($1/Å^2$)
Si – Si	Silicon-silicon bond density ($1/Å^2$)
δ_{C-C}	Percentage of C–C to Si–Si bond ratio
cF8	Cubic diamond structure ($1/Å^2$)
$cF8_1$	An atom being a first neighbor of an atom that was classified as cubic diamond. Its four neighbors are positioned on lattice sites, but at least one of its second nearest neighbors is not. ($1/Å^2$)
$cF8_2$	An atom being a second nearest neighbor of an atom that was classified as cubic diamond. The atom itself is positioned on a lattice site, but at least one of its neighbors is missing or is not positioned on a lattice site. ($1/Å^2$)
hP8	Hexagonal diamond structure ($1/Å^2$)
hP1	Graphene ($1/Å^2$)
c4	Simple cubic ($1/Å^2$)
○	Undefined structure (*i.e.* not diamond structure as identified by the diamond-structure identification algorithm) ($1/Å^2$)
$\vec{c}_d^{(q)}$	Averaged SOAP descriptor

[1] Guziewski, M.; Banadaki, A. D.; Patala, S.; Coleman, S. P. Application of Monte Carlo techniques to grain boundary structure optimization in silicon and silicon-carbide. Computational Materials Science 2020, 182, 109771, DOI: 10.1016/j.commatsci.2020.109771.
[2] Bartók, A. P.; Payne, M. C.; Kondor, R.; Csányi, G. Gaussian approximation potentials: The accuracy of quantum mechanics, without the electrons. Physical Review Letters 2010, 104, 136403, DOI: 10.1103/PhysRevLett.104.136403.

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