USC Viterbi School of Engineering

Modeling Martensite Microstructures

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Introduction

The shape-memory effect is a property of certain metal alloys in which a material appears to "remember" its original shape after a deformation. This is because the material has two phases: the rigid austenite phase at high temperatures and the more easily deformed martensite phase at low temperatures. So, no matter what shape it takes on in the martensite phase, the material will always return to the original austenite shape when it is heated. The reason why a shape-memory alloy in the martensite phase can be easily deformed is because its atoms form complex microstructures, which are the focus of my research.

Objective & Impact of Professor's Research

Professor Balakrishna's lab, the Solids & Materials Lab, studies the effects of microstructures in a variety of materials, including intercalation materials, photomechanical materials, and shape-memory alloys, using computational modeling. These insights can lead to the development of enhanced materials such as lithium-ion batteries with increased longevity.

Acknowledgements

I would like to thank Professor Balakrishna for allowing me to have this experience, as well as my mentor Delin Zhang for guiding my research and answering my questions. I would also like to thank my center mentor, Kristin Deshotel, for her help.

Citations

[1] A. Balakrishna, "Crystallographic design of intercalation materials," 2022, *arXiv:2204.04525.*

[2] K. Bhattacharya, *Microstructure of Martensite: Why it forms and how it gives rise to the shape-memory effect.* Oxford, UK: Oxford University Press, 2003.

Research & Learning Process

I learned several important concepts and skills during the course of the research:

- A matrix with positive determinant can be broken down into a stretch and a rotation.
- Each type of lattice structure has a unit cell that can be described with 3 basis vectors.
- Transformations between different lattices can be represented as a matrix transformation of the basis vectors plus a shift to the origin.

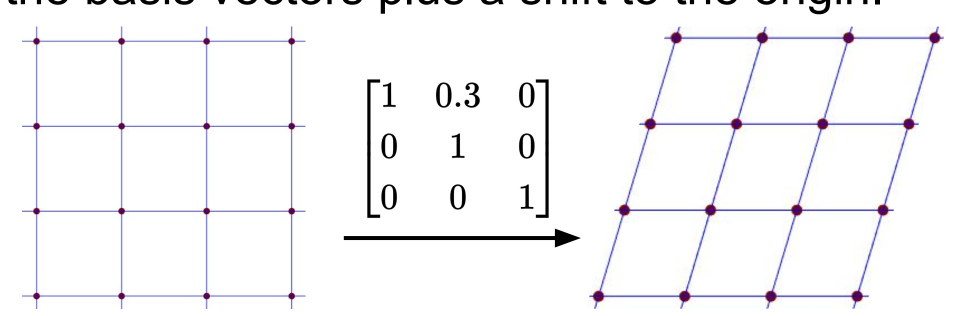

Figure 1. A 2-D cross-section of a cubic to monoclinic transformation. PC: Zahed Siddiqui

- Every lattice has a point group of rotations that do not change the overall lattice.
- A martensite lattice must have a smaller point group (less symmetry) than its austenite lattice in order to exhibit the shape-memory effect.
- Different parts of the austenite lattice can take different martensitic transformations as long as they are compatible with each other.
- The twinning equations can determine when the stretch components of two transformation matrices are compatible and if so, what rotation should be added to allow twinning.

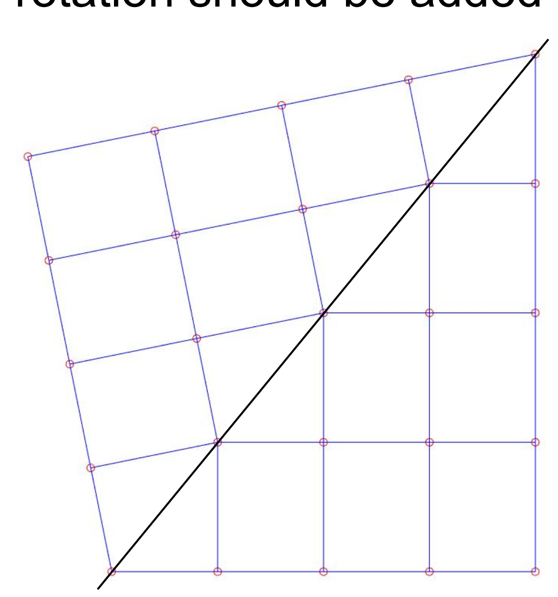

Figure 2. A 2-D cross-section of two compatible tetragonal transformations in a simple twinning system. PC: Zahed Siddiqui

- Twinning different stretch matrices together allows the martensite to have microstructure that disappears upon the transformation back to austenite.
- MATLAB's graph and network algorithms can represent the interactions between different regions in a microstructure.

Methods

Although I iterated through various methods of computing the microstructure, the final method was as follows:

1. Define the regions of the lattice and their base martensitic transformations.
2. Compute the planes at which the regions can be twinned together.
3. Create a graph structure to hold all the information about the lattice, with the nodes representing regions and the edges representing twinning planes.
4. Use the depth-first search algorithm to compute the full transformations that are applied to each region, based on the connected nodes and edges.

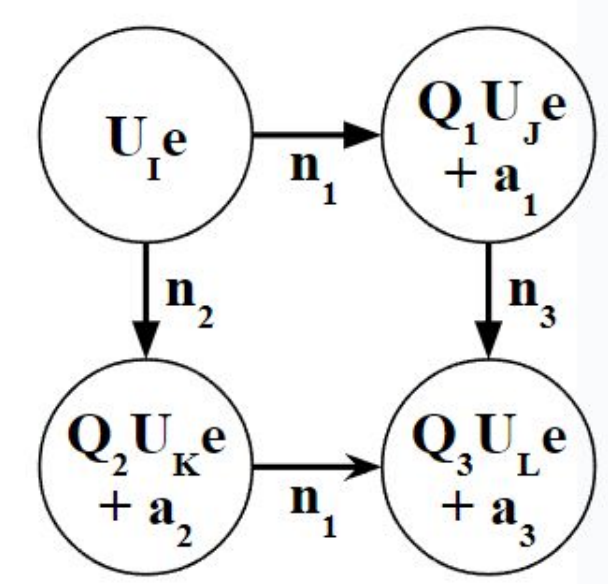

Figure 3. The graph associated with the crossing twins microstructure. Transformations are applied to the lattice vector **e**. PC: Zahed Siddiqui

5. Create a list of austenite lattice points, such that the next point in the list is always adjacent to the last.
6. Determine the region in which the first point in the list lies.
7. Find any instances when the chain of lattice points crosses into a new region by checking the twinning places associated with the edges connected to the current region's node.

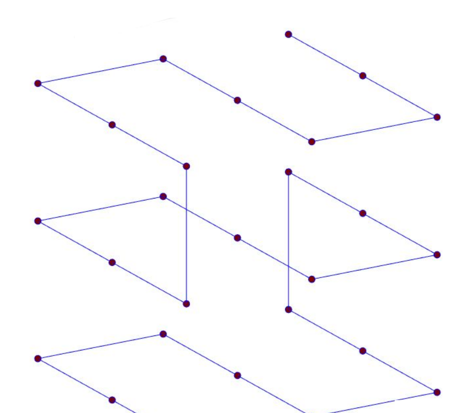

Figure 4. A single unbroken chain of austenite lattice points used by the algorithm to detect crossings to adjacent regions. PC: Zahed Siddiqui

8. Once each lattice point's region is determined, apply the corresponding transformations.

Results

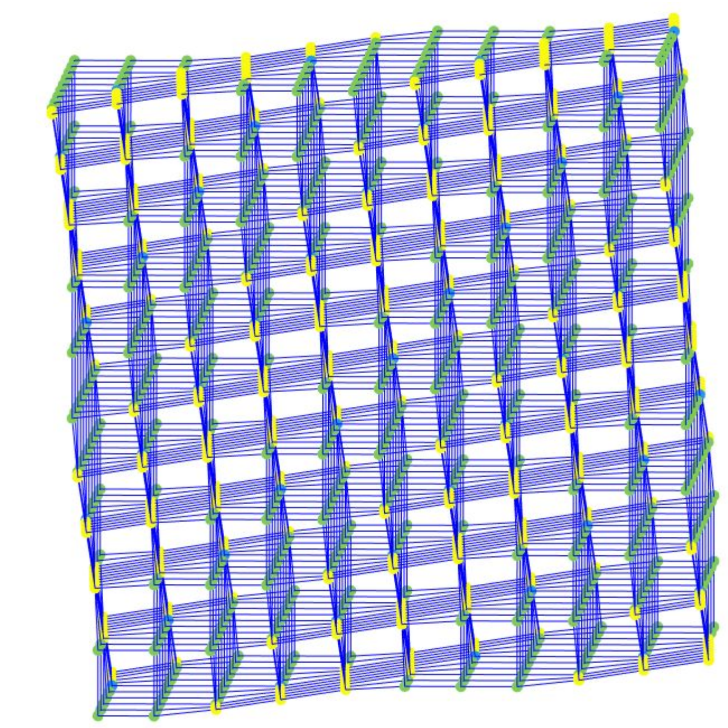

Figure 5. A microstructure of repeated parallel twins between two orthorhombic transformations. PC: Zahed Siddiqui

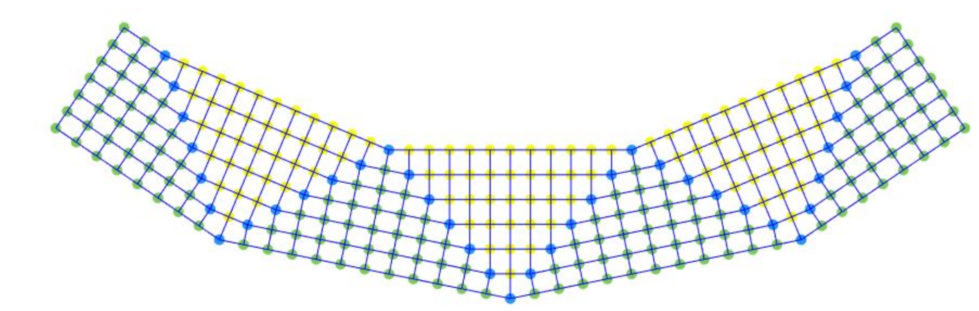

Figure 6. A microstructure of repeated twins between two tetragonal transformations in a zig-zag pattern. PC: Zahed Siddiqui

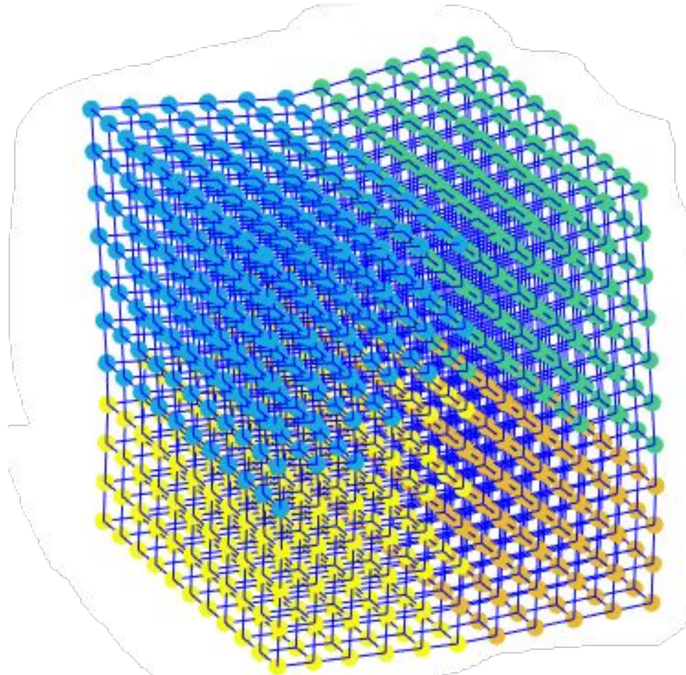

Figure 7. A microstructure of four distinct monoclinic transformations meeting at a line. PC: Zahed Siddiqui

Next Steps for You

I would like to continue the study of computational modeling in more applications and for more uses such as forecasting and optimization. I would like to find more opportunities to use these skills as they can be applicable in a wide variety of fields. Moreover, I would like to become experienced with more software for this task beyond just MATLAB, and to hopefully be able to experimentally test the results of my models.