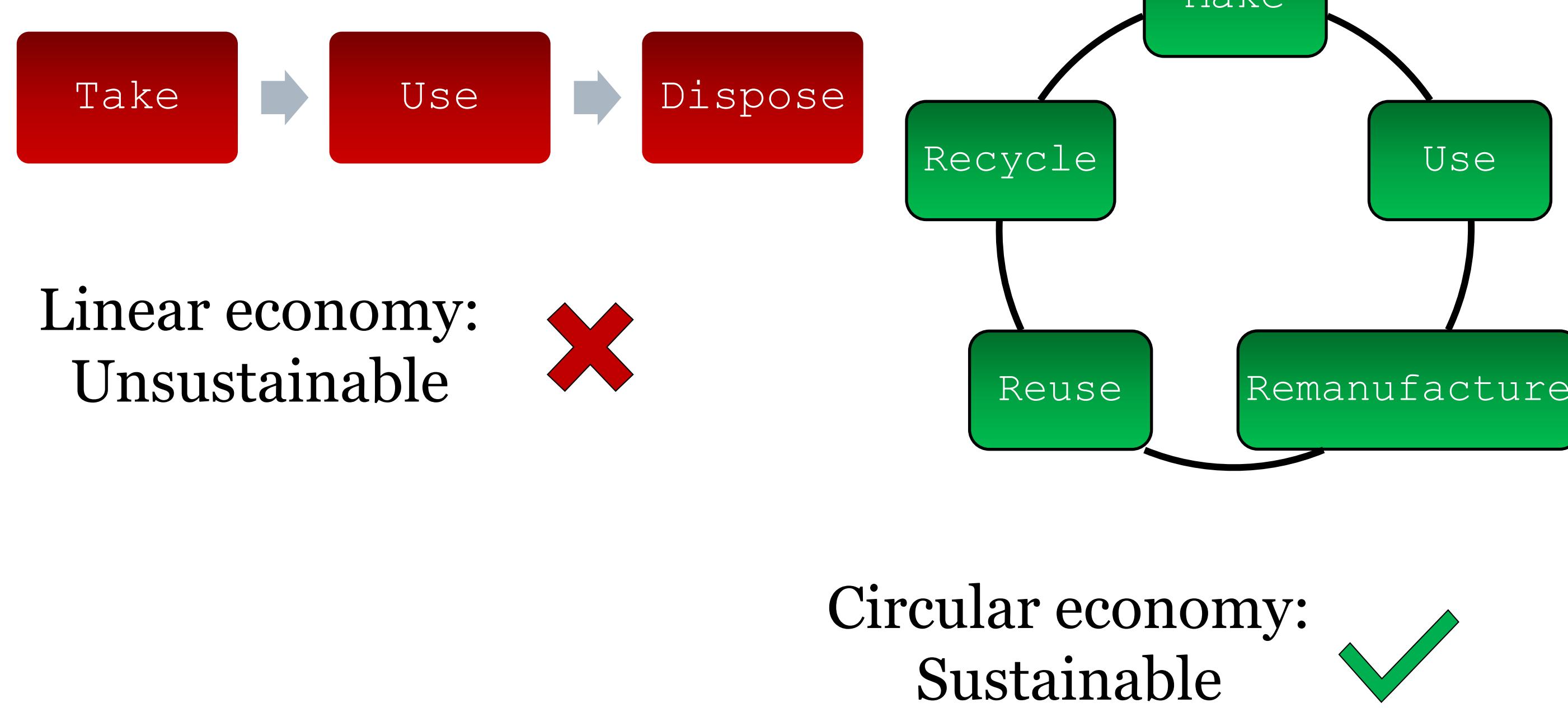


Design of Alloys for the Circular Economy

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Introduction

The circular economy focuses on the reuse, remanufacturing, and recycling of materials, including metals^[1]



- 30% of CO₂ emissions can be traced to metals production
- Computational tools are needed to accelerate development of sustainable alloys

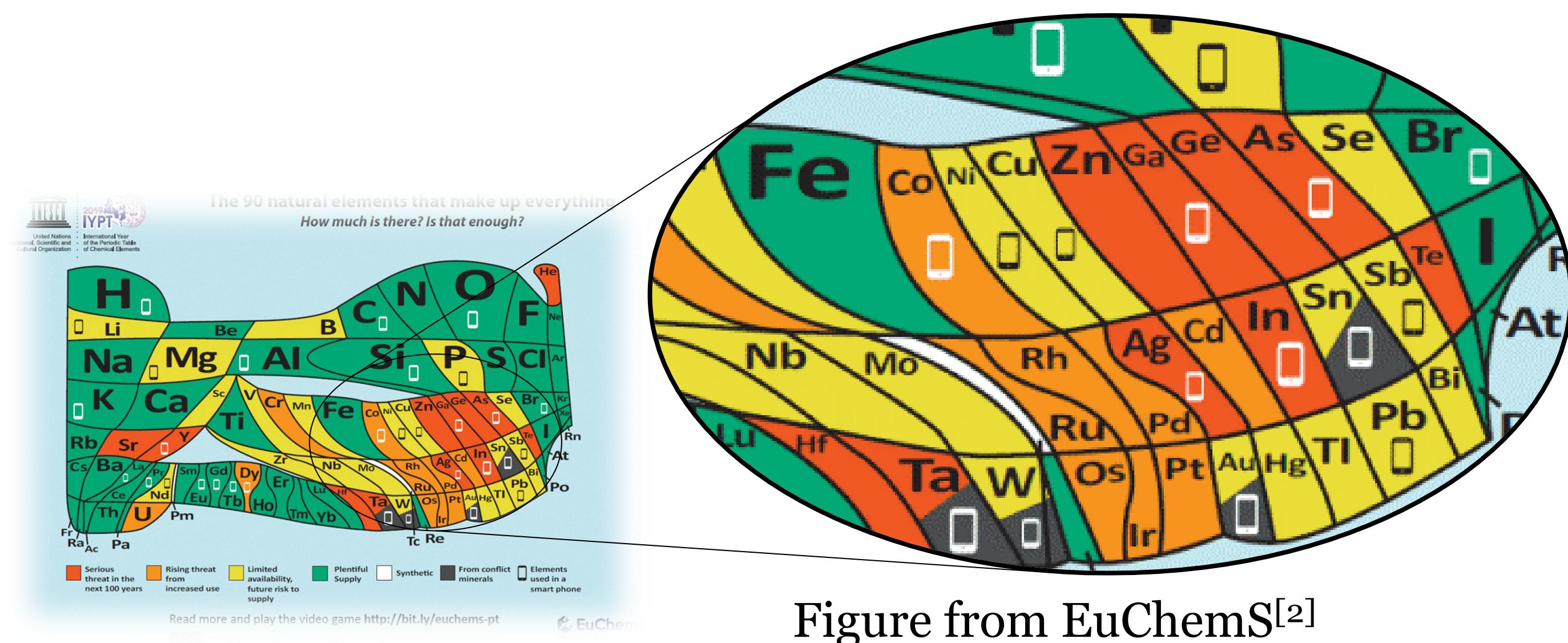


Figure from EuChemS^[2]

Materials and Methods

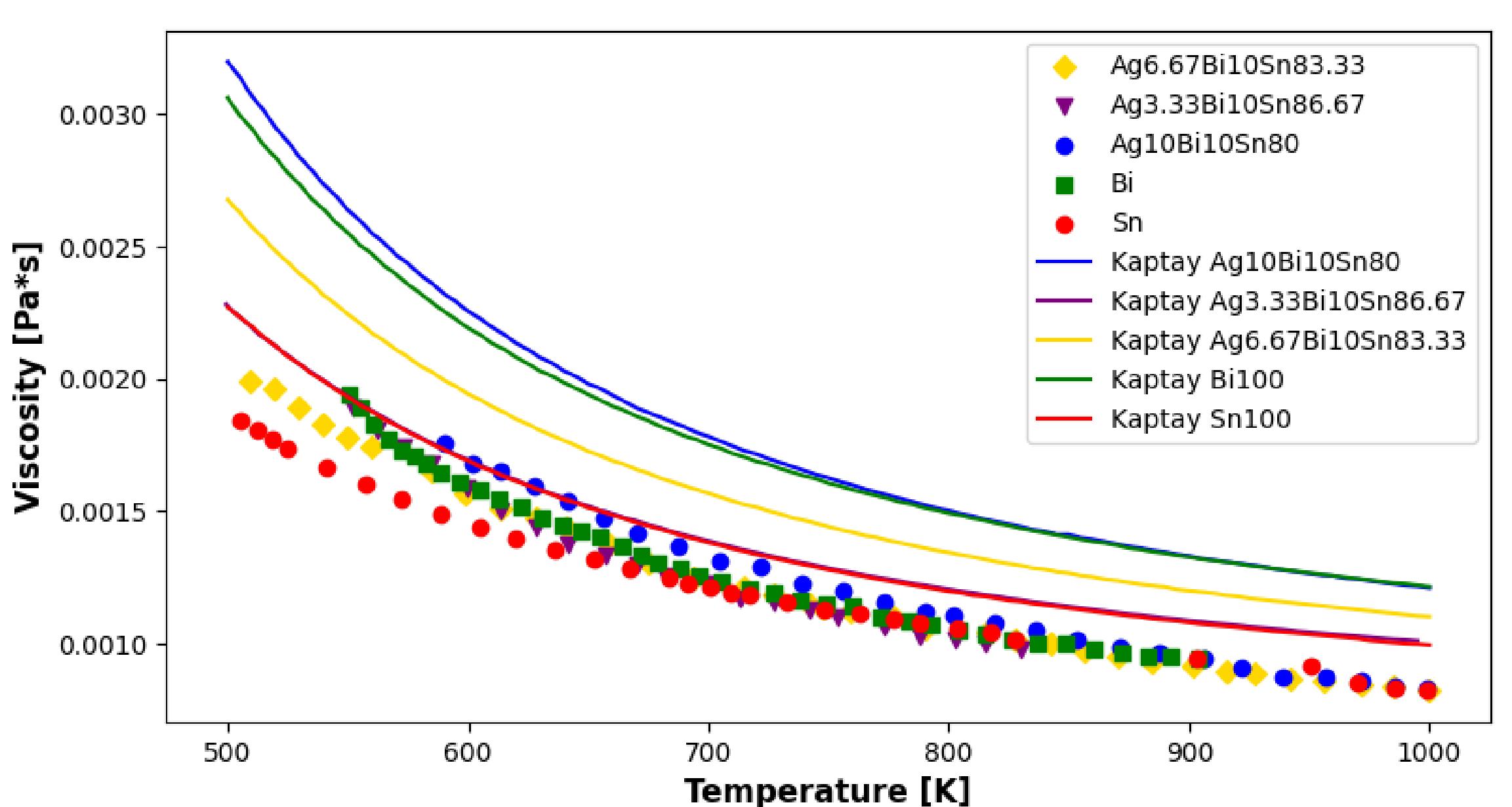


- Used to gather data, perform calculations, and plot information.
- Python was used to parallelize CALPHAD predictions with Pandat software

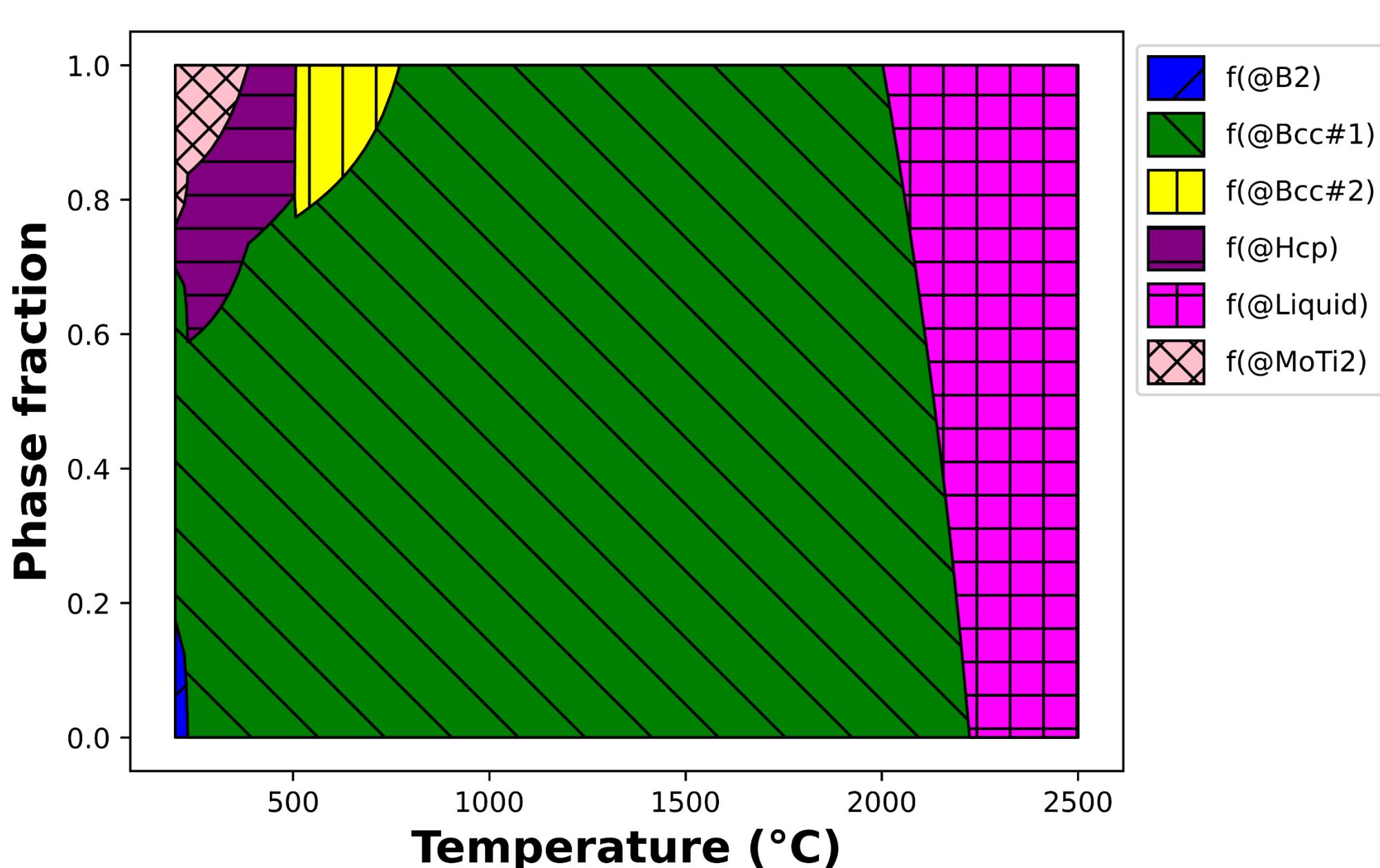


- Calculates and simulates thermodynamic, kinetic, and physical properties of alloys

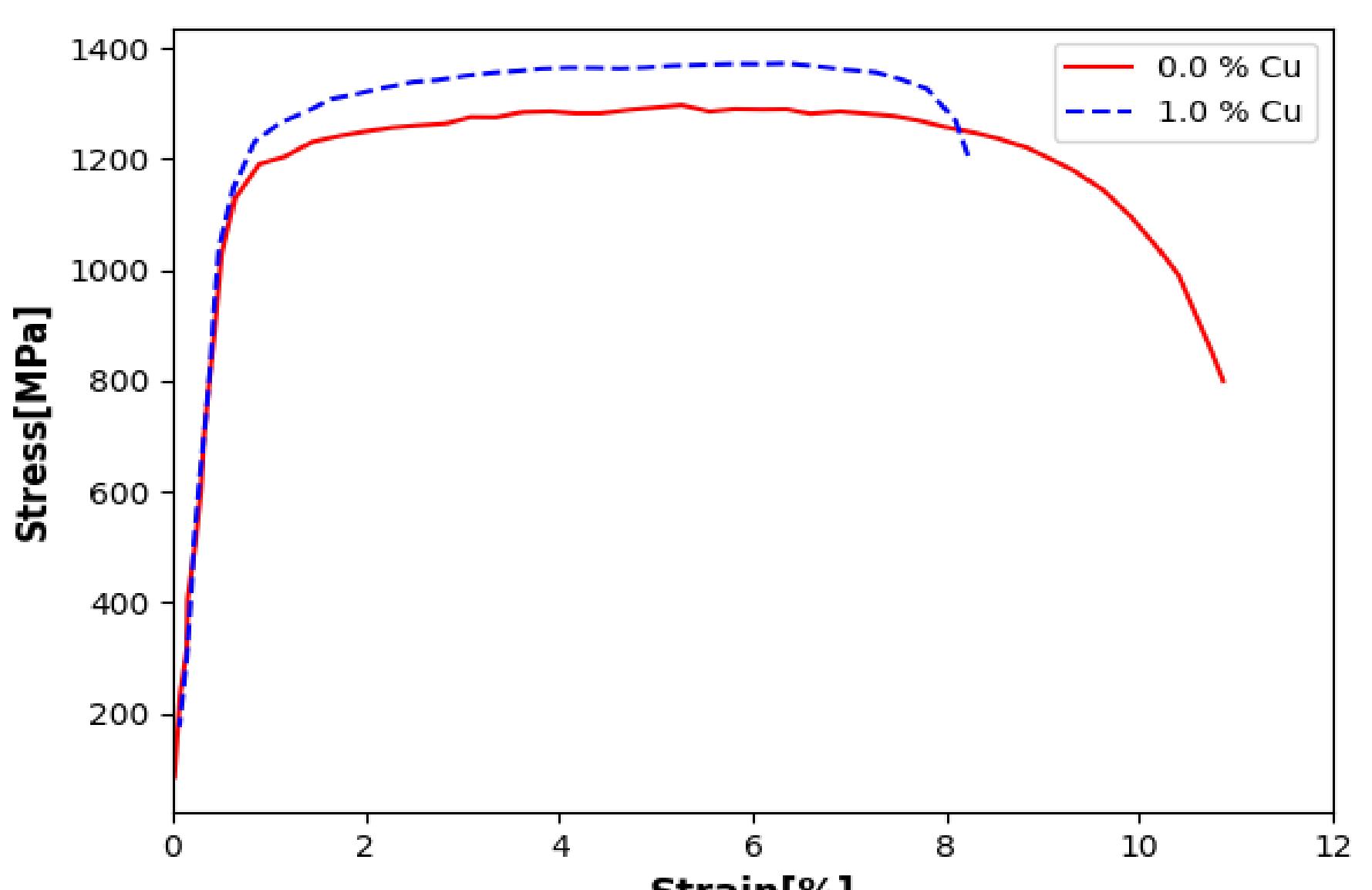
- Solidification cracking and welding behavior depends on viscosity
- Validation of my code against data from a paper for viscosity is shown below^[3]



- Deleterious phases can form in some alloy compositions
- Graph below represents each phase fraction to see if these phases might form and at what temperature

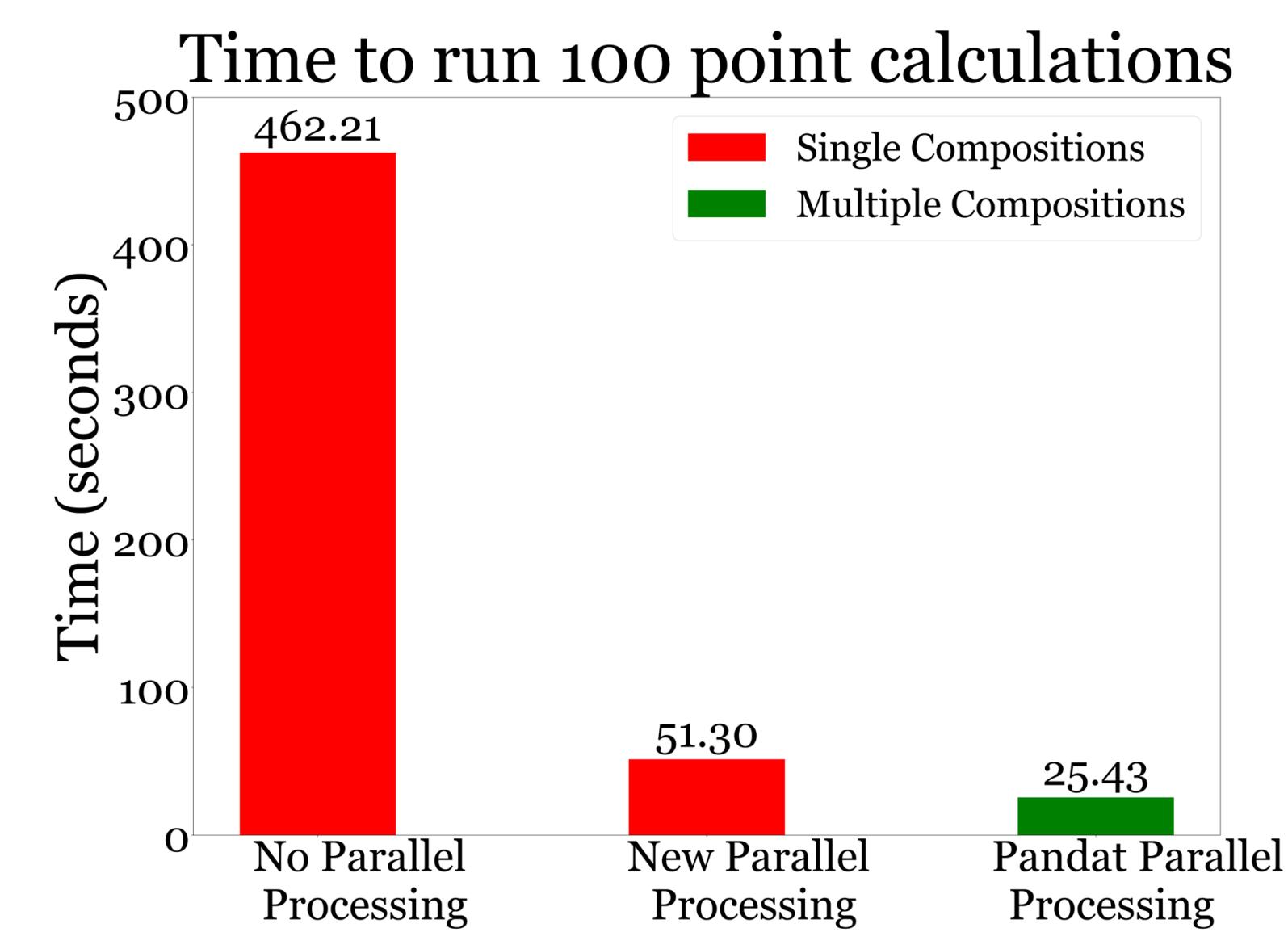


- Cu can be harmful to the integrity of steel and make it more brittle, as shown in the stress-strain diagram below^[4]



Results

- With only 72 elements, the number of 5-element systems possible is 13,991,544^[5]
- The number of systems with 3-6 elements increases to 171,318,882!^[5]
- If each calculation took 30 sec, which is very quick, it would take approximately 171 years
- Multiprocessing in Python can reduce the computation time by up to 94.45%



Conclusion

- Automation is important due to large composition space
- Property prediction models can help understand corecyclability and acceptable contaminant levels
- Future work: Use the computational tools we developed to design new alloys

References

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