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Dr. Eric Payton

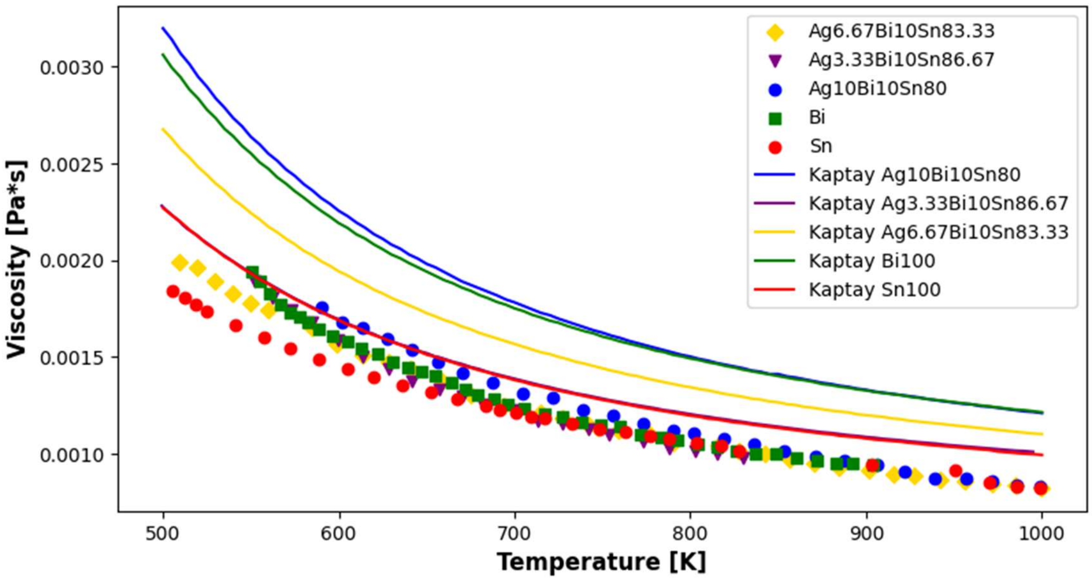
“Design of Alloys for the Circular Economy”

This summer, I took part in the project labeled “Design of Alloys for the Circular Economy,” which was led by Dr. Eric Payton. The circular economy shifts away from using materials, such as metals, for disposable products and instead focuses on using them for products that can be reused, remanufactured, and recycled. Previous work in this area includes the observation of alloy’s properties and how they change in response to their external conditions. Prior research in this area has led to the development of numerous property prediction models. As for the lab that I worked in, research has been conducted by both Dr. Payton and other students towards the design of recyclable and reusable alloys. The motivation for my work is to further the research into the design and development of new alloys for use in the circular economy.

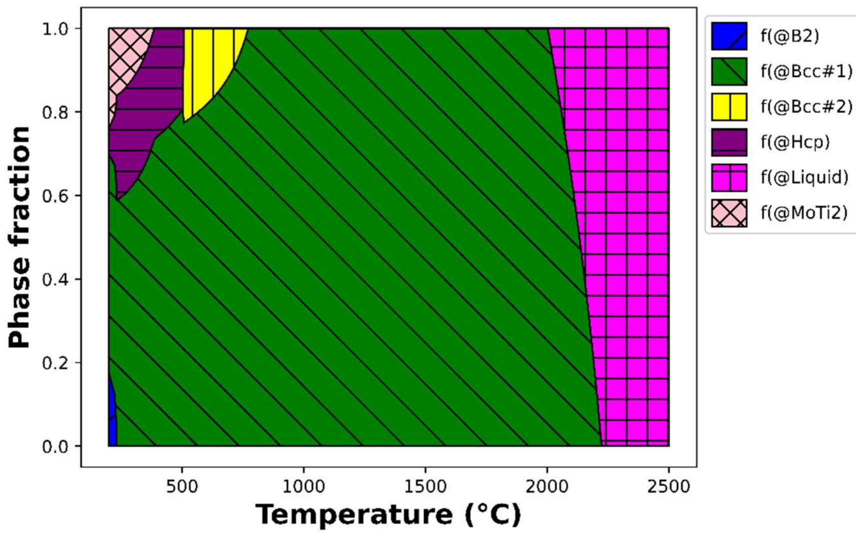
My main goal of this project was to use the coding language Python and the software Pandat to gain a better understanding of certain properties of alloys, as well as to use property prediction models and other resources to calculate and visualize these properties. These properties include the phases that are present in alloys as well as the viscosity of alloys, and they are affected by conditions such as temperature and pressure. The design of sustainable alloys is necessary for a number of reasons. First, 30 percent of carbon dioxide emissions can be traced back to metals production[2], and many elements used for alloys are of limited availability (or are at future risk of limited availability)[1], so in order to both reduce carbon dioxide emissions and limit the additional mining of already limited materials, we must develop alloys that can be reused and recycled. One personal goal that I had for this project was to help some of the grad students in my group with their personal projects (all of which relate to my project in some way), or at least to create code that will be useful for future projects in this area. I have worked towards the goals of this project by creating graphs/models that represent how physical properties like viscosity and phases of matter are affected by temperature and composition changes. Reaching a better understanding of these properties and how to measure them will allow us to make advancements toward our goal of designing new alloys. For example, being able to find the viscosity of an alloy and for a specific temperature range can help us determine how likely an alloy is to crack when it solidifies. It is important to use computational tools for the process of designing new alloys because the number of alloys that can be made limits the amount of work that can be done by hand. For example, Miracle and Senkov found that with 72 alloys, the number of 3-6 element alloys that can be made is 171,318,882[5]. With this number of alloys, it is impossible to complete by hand the calculations required for each alloy. Because of this, we must develop new computational tools that can expedite this process.

For this project, I used the open-source programming language Python along with the software Pandat to complete my objectives. I used Python to gather information from both Excel and Pandat, perform calculations, and visualize data. I also used Python to parallelize CALPHAD (calculation of phase diagrams) predictions with Pandat software. Pandat calculates and simulates thermodynamic, kinetic, and physical properties of alloys. These predictions are useful in assessing whether alloys can be co-recycled or will act as detrimental contaminants in the recycling process. When I was developing my code, I often ran into roadblocks, especially since I do not have much coding experience. When this happened, I used resources such as the internet and the other people in my lab group to find what I needed and continue my progress. I learned about Python libraries such as NumPy, Pandas, and Matplotlib, as well as how to use them for this project. I also needed to learn how Pandat worked and how the various functions that had been developed before I joined the group worked with each other and with Pandat to gather and calculate data.

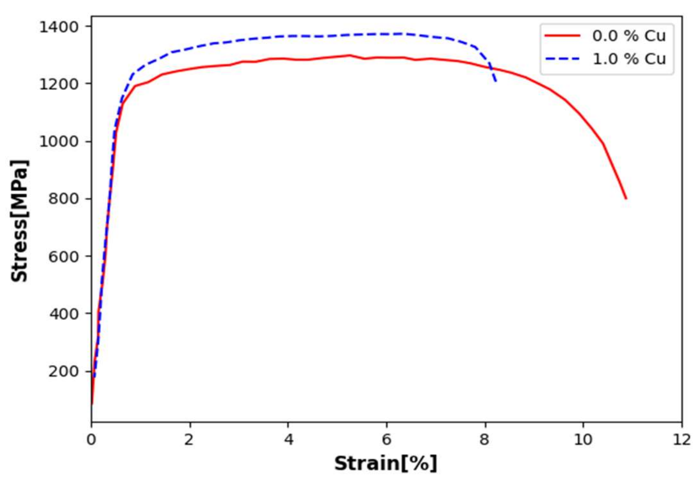
My results consist of the code I have developed for visualizing phase fractions and calculating and graphing the composition dependent viscosity. The viscosity of metals is important for many projects in our lab, but I heard the most about its importance for crack susceptibility. When metals are cast, they might crack when hardening, and this cracking depends partially on the viscosity of the alloy. The code I created both calculates and graphs the composition dependent viscosity of an alloy for a range of temperatures. An example of my code (represented by the lines) compared to experimental data[3] (represented by the shaped dots/markers) for AgBiSn alloys is shown below.



The different numbers next to each element in the legend represent how much of that element is present in the alloy (as a percentage). My code calculates the viscosity using variables such as the melting point of the alloy, which is found using Pandat, the density of the alloy, the composition of the alloy, and the temperature. For this graph, I tried to use a number of different viscosity models before finally deciding to use the Kaptay viscosity equation. First, we wanted to use the equation developed by Seetharaman and Du-Sichen, which we decided not to use because the values of certain variables were either calculated incorrectly by Pandat or were not output by Pandat at all. Another viscosity model I looked into was the Hirai model, which I ultimately decided not to use because it was not as accurate as the Kaptay model.



My next graph displays the fraction of each phase for a specific temperature range. I made this graph using the fraction of each phase present in the alloy for a certain temperature range. This means that the difference between the top and bottom of each colored section for each temperature represents the fraction of that phase present in the alloy for that temperature. This graph is important to determine whether deleterious phases (which make the alloy more brittle) will form in alloys and, if so, at what temperature(s).



This next graph is data which has been pulled from a paper written by Alexander Gramlich[4]. It shows the harmful effects that copper has on the integrity of steel. As seen in the figure, even a small amount of copper can greatly affect the amount of stress that the steel can handle. This can also occur with other metals and alloys, which is why it is important when recycling metals to regulate the number of contaminants.

Finally, it is important to use computational tools for the design of new alloys because of the large composition space mentioned earlier. Using computational tools such as multiprocessing in Python to perform several calculations at once can help us reduce the time it takes for calculations to run.

Because of the large composition space, automation is necessary for the design of new alloys. Thankfully, property prediction models can help us better understand co-recyclability and acceptable contaminant levels. In the future, I suggest that the computational tools that we have developed be used for the design of new, more sustainable alloys.

Acknowledgements

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References

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