The Effect of Copper Impurities on the Mechanical Properties of Recycled Steel

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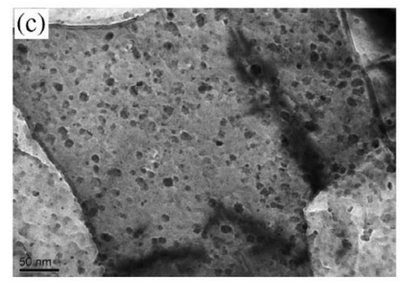
Project Background

Recycled steels often accumulate copper contaminations, which can lead to negative mechanical properties such as hot shortness [1], which is when the steel cracks at hight temperatures when it is being formed. However, it has also been shown [1] that copper can improve the strength of steel by forming a solid deposits, which are dispersed throughout the grains of the steel. These are known as precipitates. The aim of this project was to model the precipitation process and compare different strengthening models with data from literature. If accurate the model could potentially be used to set the optimal temperatures and times for the precipitation hardening process to achieve a target strength.



Bright field image of Copper Precipitates in retained austenite [8]

Research

Precipitation involves 3 stages: nucleation, growth and coarsening. [2]. These 3 stages occur somewhat simultaneously, however since we are interested in the final size of the precipitate, we focused on modelling the coarsening, with the assumption that all precipitates would end up the same size.

Coarsening follows the Ostwald Ripening process [3]: whereby smaller particles are absorbed by larger particles as a way of minimising energy. This can be modelled by LSW Theory [3], which led us to deriving the following differential equation for a precipitate, which accounts for the change in solubility as the radius increases by accounting for the Gibbs-Thompson effect [4]:

$$\frac{dr}{dt} = \frac{kr^2 e^{\frac{a}{r}}}{3r^4 + tkae^{\frac{a}{r}}}$$

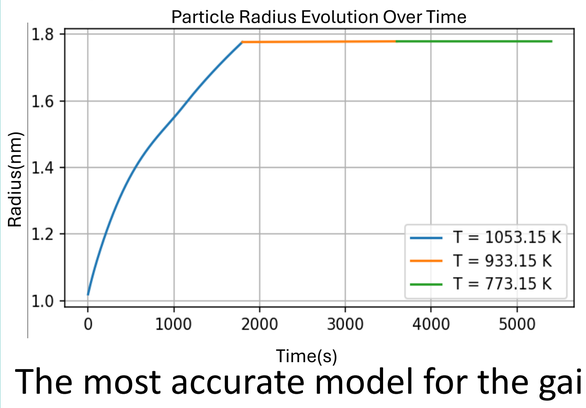
$$k = \frac{8\Gamma\Omega^2 D C_\infty}{9RT}, \qquad a = \frac{2\Gamma V}{k_B T}$$

r = radius of precipitate
t = time
Γ = interfacial energy
Ω = molar volume of precipitate
D = diffusion coefficient
C_∞ = solubility limit
R = Ideal gas constant
T = Temperature
V = Volume of an atom of the precipitate
k_B = Boltzmann Constant

Once the temperature and time was set as per each paper, the final radius of the precipitate was plugged into three strengthening models for Tensile Stress (Orowan[5], Ashby-Orowan[6], Jackson-Reed[5]) and one for Yield Stress (Russel-Brown[7]).

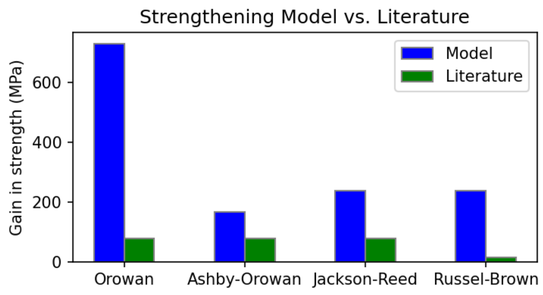
Results

One of the studies we modelled was compared to involved a 1.04wt% Cu "Transformation Induced Plasticity" (TRIP) steel which was processed in a 3-stage heat treatment [8]:



Critical radius was found to be 1.02nm as per [2] and used as the initial radius for the calculation. The final diameter was found to be 3.56nm. However, this was less than the observed value of 10-15nm.

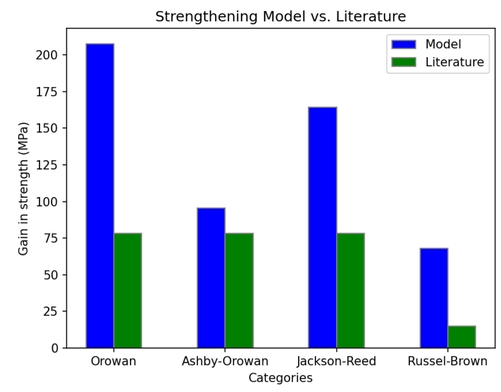
The most accurate model for the gain in strength was the Ashby-Orowan, although this too over-predicted the tensile strength by a factor of 2.15.



Discussion

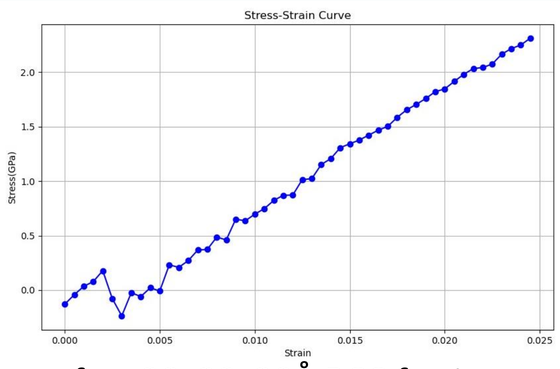
The reason behind the underestimation of final radius was likely due to an underestimation of the solubility limit. The final radius was sensitive to this parameter (for example doubling solubility increases the final radius by a factor of 1.17). The main literature that was found on the solubility of copper in iron was the following paper [9] where an empirical model was created. However, this model was derived after testing a steel with a higher Cu composition at 1.4wt% and for a temperature range of between 400-700℃, whereas for the study above the maximum temperature was 780℃.

This would have let to an underestimation of the final radius leading to an overestimation of the gain in strength. However, if we input the mean observed radius of 6.25, there is clearly a much closer correlation with the Ashby-Orowan model.

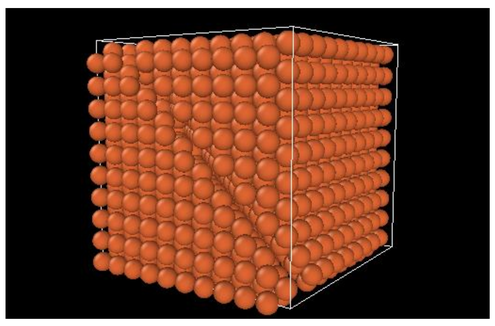


Molecular Dynamics

Molecular dynamics simulates the motion of individual atoms. The software used was LAMMPS and the final goal is to simulate precipitate-dislocation interaction.



So far, we have run a simulation of a perfect 20x20x20Å BCC ferrite lattice under a tensile stress test giving a Young's Modulus of 107.68 GPa, making it close to the expected value of the Young's Modulus of steel, 200GPa.



10x10x10Å cube with dislocation

Additionally, we have created a dislocation in a smaller cube, and we will run a tensile stress test on it as well. Then we will add the precipitate to see the difference in strength so we can compare it to the strengthening models. We may even be able to see if there is any difference between BCC, 9R and FCC precipitates.

Conclusion

The results of this study can be useful for steelmakers to predict the mechanical strength of recycled steels with a known level of copper contamination. The main success of this study was finding the Ashby-Orowan model was most the most suitable and demonstrating that LAMMPS can be used to verify our models. The focus of further study would be to consider the change in volume fraction dissolved copper as precipitation occurs and consider solution strengthening into our model.

References

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