Mechanical response of sodium silicate glass

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Abstract

We propose a new method using coarse-graining and molecular dynamics to calculate structural and mechanical properties for sodium silicate glasses at different scales. Using this method we were able to describe the mechanical behavior of the material, this way a new constitutive model was developed which could be used in continuum calculations.

Keywords: multi-scale, coarse-grain, sodium-silicate, plasticity

1 Introduction

Understanding the relationship between mechanical and structural properties is a challenging task in silicate glasses which are more and more used as structural materials.

We used classical MD simulations to analyze the mechanical response of sodium silicate glasses. The initial samples were generated by the random deposition of the atoms, the system was equilibrated at 3000 K then the kinetic energy was completely withdrawn (0 K). To model the interactions the well-known BKS potential [1] was used with partial charges. The parameters were set according to the work of Yuan and Cormack [2]. The cutoff was fine tuned to achieve the experimental densities.

The samples were compared to experiments such as neutron diffraction, NMR and Brillouin scattering measurements.

The systems were tested by deforming the periodic simulation box in a homogeneous way. During compression or tension the dimensions of the simulation box was reduced by a constant displacement step while the positions of the particles were rescaled in a homogeneous way. After the box displacement a new equilibrium position was searched using the Polak-Ribiere conjugate gradient algorithm. The shear deformation was done similarly by tilting the simulation box.

Our principal aim is to describe the effect of sodium on the mechanical properties of sodium silicate. Therefore we have divided our analysis into three major parts. In the first section the initial, linear elastic response is studied then the deformation is going to be increased until the material plastifies. Finally using the atomic scale results we define constitutive relations for continuum calculations.

2 Elastic response

The elastic stage was considered until the deformation reached 1% strain. To calculate local and global stiffness properties we used a new method allowing us to overcome finite size effects. Six different loading cases were conducted to compute the 21 elastic constants (with an over determined linear equation system). Local stresses and strains were calculated using coarse-graining technique [3]. With the local stress-strain relations we were able to compute local elastic properties (detailed in the Ref [4]). Using these results we established a spatial correlation between the distribution of sodium and the local stiffness of the material. We found that sodium rich regions have a direct effect on the reduction of the materials Young's and shear modulus.

3. Plastic response

The analysis of the plastic response showed that not only the composition but also pressure can change the elastic response of the material, however not affecting the plastic plateau significantly.
We showed that by adding sodium into silica systems the elastic yield strength reduces and the softening behavior disappears, the material plastifies in an early state entering the plastic plateau quicker.
The local stress-strain behavior showed us that low sodium content materials have a clearly elastic response at low pressure, but entering a densification stage the local structure collapses and the occurrence of local shear rearrangements at low shear strain value is facilitated by the soft spots in the material. Therefore the elastic stage disappears and the material enters a plastic plateau much more easily at 5 GPa than at -2 GPa.

4. Constitutive relations

By registering the remaining shear and volume deformation in the function of the applied stress state we can draw conclusions about the ductile behavior of the material and construct yield surfaces which then could be used in continuum simulations. This way we can test the material sufficiently using simulation which could be difficult in microscopic experiments. If we draw the remaining volume and shear strain in the function of pressure and shear stress we can construct the hardening yield surface.

5. Conclusion

We found molecular dynamics a very valuable tool to mechanically test materials at the micro-scale, where experiments are usually limited by the size of the sample. We were able to explain the macroscopically observed transition between different compositions and pressure states using local stress and strain analysis. Using the constitutive model developed in MD we are able to step on a higher scale, and using finite element methods should allow us to compare experimental results with continuum numerical calculations.

References

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