Young's modulus prediction for oxide glasses assisted by machine learning

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Abstract

Glass has been known for thousands of years and used in many fields such as housing, packaging, automotive, aeronautics, telecommunications, and cosmetics. This material is sustainable, although it requires a lot of quantity of energy, and it is a product with eco-responsible characteristics. It is chemically neutral and impermeable to gases and can be recycled ad infinitum without altering its composition or properties. Plastic is a material that is used in many areas. Its particularities make it a low-cost, resistant, and easy to produce in large quantities. Despite many qualities, it is also very polluting. For ecological reasons, we want to replace plastic packaging with glass, while maintaining the same characteristics (weight, mechanical resistance).
In addition, reducing the weight of glass packaging leads to a reduction in raw materials, but also to a significant environmental impact. Lightweight glass is one of the challenges of our time to reduce the carbon footprint of industry. Despite the extensive use of oxide glasses in industry, the composition-property behaviours of these materials are still poorly understood, particularly for lightweight impact-resistant glass. According to Makishima-Mackenzie model (MM) the Young's modulus of glass depends on the dissociation energy, the atomic packing fraction, and the glass density. However, for certain ranges of glass composition, predictions underestimate the experimental values, particularly in the high range. This equation provides a clear physical picture of the compositional dependence of certain physical properties such as glass hardness.

The objective of this work is first to test the existing mathematical models proposed by Makishima and Mackenzie (1973) and improved by Shi et al. (2020) on a test dataset. A similar approach has been done using a machine learning model by Ravinder et al. (2020). We develop a numerical procedure combining machine learning and physical models. The MM model shows good reproducibility for Young's modulus ranges from 40 to 80 GPa and drifts beyond this value. To improve the MM model, Shi et al. (2020) introduce the effect of compaction. However, it is only evaluated for single glass compositions containing three to four oxides. We propose an extension of the Shi et al.'s model coupling with a machine learning procedure. The aim is to increase the glass composition domain and explore unknown compositions to optimize lightweight products.

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