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Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Stepniewska, M., Zhou, C., & Yue, Y. (2017). *Fracture and Deformation Behavior of Melt-Quenched ZIF Glasses*. Abstract from 7th International Workshop on Flow and Fracture of Advanced Glasses, Aalborg, Denmark.

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Fracture and Deformation Behavior of Melt-Quenched ZIF Glasses

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Due to their notable properties and a vast range of possible application, Zeolitic Imidazole Frameworks (ZIFs) have been lately attracting a lot of attention. Recently discovered melt-quenched ZIF (MQ-ZIF) glasses as a new group of amorphous materials show a number of desirable properties, such as high thermal and chemical stability [1-3]. However, up to now, no systematised studies concerning mechanical properties and fracture behaviour have been performed on these glasses. Such studies are particularly crucial for future applications in any load bearing systems, especially those at risk of sudden cracking.

In this study, we focus on the fracture behaviour of ZIF-62, built of zinc ions connected by two types of organic ligands (namely, imidazole – Im, and benzimidazole - bIm). Two groups of samples – changing content of only one of the ligand for given group - have been prepared. By changing the ratio of ligands in the structure during synthesis, we obtained initial results showing an influence of chemical composition on material – both for the crystals formed during synthesis and the following melt-quenched glasses. Considering the different size of bIm and Im molecules, chemical composition is expected to greatly influence the structure, and hence, mechanical properties. By measuring the hardness and observing the cracking patterns of ZIF-62 glasses, we attempt to understand the structural impact on mechanical properties of ZIF-62 glasses. Initial results show a clear effect of chemical composition on the fracture behaviour and crack patterns of the samples. We observe the crack formation during indentation by using scanning electron microscopy and describe the influence of chemical composition on crack initiation and propagation. Carrying out the measurements with different loads for chosen samples also enables us to describe the scale effect visible for hardness in MQ-ZIF. In addition to that, we undertake first trials of quantifying different deformation mechanisms for indentation (densification, elastic deformation, plastic flow) with the use of atomic force microscopy. We perform structural characterisation of the ZIF-62 by nuclear magnetic resonance (NMR) and infrared spectroscopy, and find the structural origin of chemistry dependence of fracture behaviour. Finally, we also compare the fracture behaviour of MOF glasses with that of other types of glasses such as oxide glasses and metallic glasses.

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