ATOMISTIC SIMULATIONS OF AMORPHOUS METALS UNDER UNIAXIAL COMPRESSION AT DIFFERENT TEMPERATURES

Franco Ardiani[a], Andrés A. Manelli[a], Carlos J. Ruestes[b], Claudio A. Careglio[a,c] y Eduardo M. Bringa[b,d]

[a]*Facultad de Ingeniería, Universidad Nacional de Cuyo, Centro Universitario, Parque General San Martín, 5500 Mendoza, Argentina, francoamg@gmail.com, andresmanelli@gmail.com, ccareglio@uncu.edu.ar*

[b]*Instituto de Ciencias Básicas, Universidad Nacional de Cuyo, 5500 Mendoza, Argentina, cjruestes@hotmail.com, ebringa@yahoo.com*

[c]*Instituto para las Tecnologías de la Información y las Comunicaciones (ITIC) – Universidad Nacional de Cuyo, 5500 Mendoza, Argentina*

[d]*CONICET, 5500 Mendoza, Argentina*

Keywords: Amorphous metals, mechanical properties, elastoplastic strains, atomistic simulations

Abstract. Amorphous metals, i.e. without defined crystal structure, are increasingly used in modern life, showing great potential as advanced engineering materials, due to some of its characteristic properties such as high hardness and moldability, high resilence, high mechanical strength, and high wear resistance, among others. All these properties allow obtaining parts with complex shapes and high strength, which increases their chances for industrial application. However, many details of the mechanical behavior are still unknown, and the currently used models and theories are far from predictive.

One of the possibilities to determine constitutive parameters, and thus study the response of these materials, is by using atomistic calculations. In this poster we present results obtained with molecular dynamics (MD) simulations of an amorphous metal (CuZr). In particular, constitutive parameters such as the elasticity modulus, are determined for a sample subjected to uniaxial compression at different temperatures. The results obtained are relevant for understanding the mechanical behavior of the material, such as stress-strain and temperature-strain relationships.