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Molecular dynamic study of mechanical behavior of cis-PB under shock loading NICOLAS PINEAU, GAUTIER LECOUTRE, CLAIRE LEMARCHAND, LAURENT SOULARD, CEA/DAM/DIF — Using molecular dynamics to generate relaxed configuration in order to characterize the mechanical behavior of polymers is an application of great interest but require a complex methodology. First of all, we use a versatile algorithm initiated by Lemarchand and al. [1] to generate long and realistic polymer chains of cis-polybutadiene. We performed non-reactive simulations using the OPLS force-field for intramolecular interactions and the Buckingham exponential-6 potential for intermolecular interactions [2]. Under shock compression, the principal aim is to study the mechanical response quantified by Hugoniot curves and the structural properties of the chains such as the radius of gyrations, the chains orientations, the shape Using explicit shock and Hugoniostat simulation [3], we focus on the influence of different shock regimes and chain length. References [1] C. A. Lemarchand, D. Bousquet, B.Schnell, N.Pineau, submitted to J. Chem. Phys [2] Markus G. Frhlich, Thomas D. Sewell, and Donald L. Thompson J. Chem. Phys. 140,024902 114:16, (2014) [3] J.-B. Maillet, M. Mareschal, L. Soulard, R. Ravelo, P. S. Lomdahl, T. C. Germann, and B. L. Holian Phys. Rev. E 63, 016121 (2000)

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