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# Molecular dynamics simulations of structural transitions of crystalline polystyrene in response to external stresses and temperatures

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## Abstract

The structural transitions of syndiotactic polystyrene in response to external stresses and temperature were investigated in detail by molecular dynamics simulations. Upon uniaxial compression along the  $b$ -axis, the nanoporous  $\varepsilon$  form was transformed into a lower-density porous “S-I” form, accompanied by marked elongation of the  $a$ -axis. The S-I form was transformed into the  $\gamma$  form following stress reduction. The transition from the  $\varepsilon$  to the  $\beta'$  form was also observed under tensile stress along the  $c$ -axis, which is associated with a conformational transition of the main chains. The stress responses and the reproducibility of the transitions were confirmed by extensive simulations. The thermal stability of the polymorphs was also examined *via* stepwise heating simulations. Experimentally observed thermal transitions of  $\varepsilon \rightarrow \gamma$  and  $\delta_e \rightarrow \gamma$  were reproduced. It was found that the S-I form is more stable than the  $\varepsilon$  and  $\delta_e$  forms under 0.27 GPa uniaxial stress along the  $b$ -axis. Considering the reproducibility of the stress-induced transitions and the thermal stability, the S-I form could be realized under an appropriate stress condition, though no experimental observation has been reported for now.

*Keywords:* molecular dynamics simulation, polystyrene, crystal, stress

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## 1. Introduction

The crystal structure prediction from first principles is recently much interested, not only in material design but also in fundamental sciences [1, 2]. Various methods [3–7] have been proposed and tested in combination with *ab initio* calculations and molecular dynamics (MD) simulations. These methods

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