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Band structure engineering of graphene by strain[1] JIANXIN ZHONG, GUI GUI, JIN LI, Department of Physics, Xiangtan University, Hunan 411105, China — We have investigated the electronic structure of graphene under different planar strain distributions using the first principles pseudopotential planewave method and the tight-binding approach. We found that graphene with a symmetrical strain distribution is always a zero band gap semiconductor and its pseudogap decreases linearly with the strain strength in the elastic regime. However, asymmetrical strain distributions in graphene result in opening of band gaps at the Fermi level. For the graphene with a strain distribution parallel to C-C bonds, its band gap continuously increases to its maximum width of 0.486 eV as the strain increases. For the graphene with a strain distribution perpendicular to C-C bonds, its band gap continuously increases only to 0.170 eV. The anisotropic nature of graphene is also reflected by different Poisson ratios in different directions. We found that the Poisson ratio is 0.079 and 0.255 for the strain distributions parallel to or perpendicular to C-C bonds, respectively. These findings are important for understanding and controlling the transport properties of graphene systems.

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