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A Study on Mechanical Behaviors of GaP Nanowires by Molecular Dynamics Simulation

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Mechanical and fracture behaviors of GaP nanowires (NWs) in zinc-blende and wurtzite phases were investigated by Molecular dynamics simulations using the program package LAMMPS with Tersoff potential. Simulation was performed and focused on the effects of different structure, orientation, length, temperature and diameter on the behaviors of slip system, strength, stress distribution and fracture mechanism of NWs under uniaxial tension. Simulation results show that the magnitude of Young's modulus of zinc-blende GaP NWs in [111] orientation is greater than [110] and [001], while it is the smallest in [001]. For zinc-blende [111] and wurtzite [0001] GaP NWs with different cross-sectional shape, the magnitude of Young's modulus of square is higher than the hexagon. On the other hand, the size effect of the NWs within the range from 2.7 to 5.7 nm in diameter is significant. The magnitude of Young's modulus and fracture stress of zinc-blende GaP nanowires decreases with the decrease of diameter. However, the magnitude of Young's modulus and fracture stress of wurtzite GaP nanowires has no such a monotonic relation. In addition, the fracture stress of both zinc-blende and wurtzite GaP NWs increases with decreasing temperature and strain rate but with increasing length of NWs. The fracture of zinc-blende and wurtzite GaP NWs is initiated individually from the corner and the side of the outer surface on a specific cross section. Specially, the strength of the NWs in wurtzite structure is higher than in zinc-blende structure.

Biography

Professor Tei-Chen Chen was graduated and received his B.S., M.S. and Ph.D. degrees in mechanical engineering from National ChengKung University (NCKU), Tainan, Taiwan, R.O.C., in 1975, 1977 and 1988, respectively. He worked at China Steel Cooperation, Kaohsiung city, Taiwan, from 1979 to 1983, and then moved to the NCKU. Now he is a Professor in the Department of Mechanical Engineering, NCKU. He has published over 100 technical papers in the area of analysis of thermal stresses, nanotechnology, inverse problems, metal forming, IC packaging, growth of single crystal, and properties of thin film layers.