

Abstract Submitted
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Effects of Sc-doping on the structure and physical properties of AlN: first-principles studies¹ CHENGXIN WANG, ZHIFAN WANG, Chengdu Green Energy and Green Manufacturing Technology RD Center, YANNING ZHANG, University of Electronic Science and Technology of China, CHENGDU GREEN ENERGY AND GREEN MANUFACTURING TECHNOLOGY RD CENTER COLLABORATION, UNIVERSITY OF ELECTRONIC SCIENCE AND TECHNOLOGY OF CHINA COLLABORATION — It was found in experiments that Sc doping can significantly improve the piezoelectric property of wurtzite AlN, making AlN_{Sc} compounds promising in the applications of piezoelectric acoustic device. However, the piezoelectric constant of Al_{1-x}NSc_x drops quickly if the Sc doping content is larger than 43%, probably due to the phase transition of Al_{1-x}NSc_x.^{1,2} In this work, we performed systematic first principles calculations on the structural, mechanical and physical properties of Sc-doped AlN, as a dependence of Sc compositions, so as to understand how the Sc-doping affects the properties of AlN. The calculated lattice parameters and piezoelectric constant corresponds well with the experimental data, reaching to the peak at $x = 43.5\%$. Also we found that with the increasing Sc contents, the elastic constants of C_{33} , C_{11} and C_{44} decrease, whereas C_{12} and C_{13} increase. The total energy calculations show that Al_{1-x}NSc_x with a wurtzite phase is more stable than the rocksalt phase as $x < 31.25\%$, and then the rocksalt Al_{1-x}NSc_x that has few piezoelectric property is energetically preferred. Ab-initio molecular dynamic (AIMD) studies were further employed to analyze the phase transition of Al_{0.5}NSc_{0.5}. 1. A. Morito, K. Toshihiro, K. Kazuhiko, T. Akihiko, T. Yukihiro and K. Nobuaki, *Advanced Materials* **21**, 593-596 (2009). 2. O. Leon, A. Morn and R. Gonzalez, *Applied Physics Letters* **95**, 162107-162107-162103 (2009).

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