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ABSTRACT

First-principles modeling of OTS chalcogenides for SELECTORS

Density Functional Theory calculations show that the nature of the mobility-gap states in amorphous Ge-rich Ge50Se50 is related to Ge-Ge bonds, at discrepancy with generally-accepted picture of valence-alternating-pairs (VAP) in chalcogenides. The use of hybrid exchange-correlation functionals is not enough to obtain a faithful description of the electronic structure – disorder-induced Anderson-localized states extend up to 1.5-2nm, which imposes a minimum size on the simulation models, if accurate mobility-gap is required. Electric field has a great impact on the state energy and localization in space. This could be an important factor for threshold switching mechanism. OTS materials undergo significant changes during ageing. Qualitative theoretical understanding of material ageing can explain the observed reliability of the prepared selector devices: a reduction of less exothermic Ge-Ge bonds in favor of the more exothermic Ge-Se bonds reduces the amount of charge traps in the system, which leads to coordination changes, mobility-gap increase and subsequently increasing the threshold voltage (Vth) and reduced leakage current (Ioff).

BIO

Dr. Sergiu Clima is a Principal Scientist at IMEC, Belgium. He received his M.S. and PhD degree in Computational Chemistry at KU Leuven, Belgium, in 2003 and 2007, respectively. Later that year he joined the Modeling Group at IMEC as First-Principles Simulations Researcher. His research activities include Density Functional Theory simulations for electronic devices: the selection of next-generation high-κ materials for DRAM MIMCAP, the fundamental understanding of the working principles of transition-metal-based emerging RRAM, FLASH, FEFET memories and OTS chalcogenides.