Ab initio study of structural, electronic and magnetic Properties of transition metals disilicides CoSi$_2$ and NiSi$_2$

Sonia.OUCHENE, NasrEddine DERRADJI, Mohamed.Tahar. KADRI, Hafid BELKHIR
Laboratoire LESIMS, Département de Physique, Faculté des Sciences, Université Badji Mokhtar (Algérie)
nederradji@yahoo.fr

Transition metal (TM) silicides, due to their technological importance, have incited over the past years numerous studies on their electronic and structural properties, both experimental and theoretical [1–2]. These compounds show stability of both, their crystalline and electronic properties at high temperatures [3]. Which make them in silicide/Si heterostructures in CMOS technology [4, 5], applications in nanoscale wires [6] or in technology of emitter tips for using in vacuum silicide-coated/silicon devices, to be implemented in flat panel displays [7], amongst several other applications. More recently, investigations have been devoted to the understanding of magnetic properties of TM silicides multilayers, mainly in relation to possible applications in the field of magnetoresistance [8, 9]. For this reason, basic research about the magnetic properties of TMS is a current issue of interest in the fields of Physics and Surface Science, in order to improve further technological performances. In this work we present a theoretical study for a system of a system Co–Ni silicides, which crystallize in the fluorite structure, they have a low resistivity (~50 and ~20 $\mu\Omega$/cm, respectively [10]) and display good lattice matching to silicon (0.46% and 1.2% [11]), so that integration in silicon matrices could be possible with negligible strain and defect formation. Therefore, the aim of this paper is to provide a study of structural and electronic properties and a prediction study of the magnetic properties of CoSi$_2$ and NiSi$_2$ using the full-potential linearized augmented plane wave (FP-LAPW) method.

Keywords: DFT, Electronic property, Magnetic property

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