Description for the general public

In spite of big advances in semiconductor physics and technology (III-V, II-VI compounds) Si and Ge (group IV) are still leading materials in integrated circuits and electronic devices industry. The reason is a long experience in the production of the devices, well established technology and low costs. This fact, in connection with challenges of modern optical fiber telecommunication (the need for light emitters and detectors) stimulates searching for materials which, on the one hand, can be easily integrated with Si and Ge and, on the other hand, have properties suitable for optoelectronics, like high effectiveness of photoemission or high mobility of carriers. Unfortunately, both Si and Ge have indirect band gap causing low effectiveness of radiative recombination. It is known however that some modifications of the materials, consisting in addition of other group IV elements and/or inducing strains can lead to appropriate changes in their electronic structures. Discovery of such modified materials which could be integrated with Si technology would be a very precious contribution to the development of modern telecommunication technologies.

The aim of the project is to **identify materials** among Ge-IV alloys which would be suitable for applications in optoelectronics, as light emitters or detectors. The choice of the class of materials (Ge-IV alloys) has been determined by the possibility of integration with Si technology, a leading one in integrated circuits (CI) and semiconductor devices industry. The need for semiconductor light emitters and detectors, in turn, is stimulated by the development of optical fiber telecommunication.

The hypothesis we intend to prove is that among a vast number of various systems from the Ge-IV group there are materials of very good optoelectronic properties. There some premises that the hypothesis is true, e.g. it is known that $\mathbf{Ge_{1-x}Sn_x}$ **,** in some range of compositions poses direct band gap in the infrared range and high mobility of carries, however the knowledge of the systems is very incomplete. We plan the systematic investigations of binary systems, $\mathbf{Ge_{1-x}C_x}$**,** $\mathbf{Ge_{1-x}Sn_x}$**,** $\mathbf{Ge_{1-x}Pb_x}$, all belonging to the class of highly mismatched alloys (HMA), characterized by a large bowing of the band gap. The effect of isotropic and biaxial strain will be also investigated. Then, the effect of admixture of other elements will be considered (**ternary and quaternary Ge-IV systems**). As a result we expect to gain a systematic knowledge about physical properties of the systems which are important for optoelectronic applications (geometric parameters, electronic structures, band gaps, band offsets, effective masses etc.).

The methodology used in the project are large scale quantitative theoretical calculations from first principles based on density functional theory (DFT). The method is known for its **predictive power**, i.e. it is possible to evaluate various quantitative characteristics of materials (structural, elastic, electronic and other) relatively quickly and at low costs. The investigations will be conducted in a close collaborations with the Experimental Physics Department at Wroclaw University of Technology where the systems will be investigated experimentally. Verified in this way calculations will become a priceless source of information about unknown materials of potential applications in optoelectronics.