PhD Proposal 2017

School: ECL	
Laboratory: INL	**Web site:** http://inl.cnrs.fr/
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Title: Nanostructured thermoelectric oxide films integrated on silicon for on-chip thermal management
Scientific field: materials science, physics, inorganic chemistry
Key words: thermoelectrics, oxides, $SrTiO_3$, films, nanostructures, phononic engineering

Details for the subject:

1. Background, Context:

Nowadays, thermal management has become of major importance in microelectronic devices since compactness and working temperatures are increasing. Either device temperature has to be controlled / reduced in order to obtain acceptable efficiency (*e.g.* laser) or waste thermal energy could be harvested and converted into electricity to build autonomous devices. Thermoelectric (TE) materials allow reaching both objectives: (*i*) temperature control or cooling by *Peltier* effect or (*ii*) harvesting waste thermal energy and making an electrical generator by *Seebeck* effect [1]. However, the main challenge of TE efficiency is to use materials having both high electrical conductivity and very low thermal conductivity (in order to maintain a significant thermal gradient across them). Maintaining a significant thermal gradient across the TE material is even more challenging in films when integration in compact microelectronic devices is targeted. Phononic strategies based on nanostructurations are promising in this view [2]. Moreover, thermoelectric materials have to be non toxic, chemically stable and abundant (thus cheap). Today, the main thermoelectric materials working around room temperature are based on Bi_2Te_3 and Sb_2Te_3 [1], which are toxic, chemically unstable and expensive because of scarcity. There is thus an obvious need to develop alternative thermoelectric materials that respect these specifications. Thermoelectric materials based on oxides are good candidates, especially single-crystalline oxide films based on $SrTiO_3$ (STO) in which electrical conductivity, Seebeck coefficient, and phononic effects can be large and tuned by doping and nanostructuration [3-4]. Moreover, this material of perovskite structure can be epitaxially integrated (in single-crystalline films) on microelectronic platforms based on Si by molecular beam epitaxy (MBE) in which the team has a long-term internationally recognized expertise [5]. The interfacial contact resistances with electrodes in *p-n* legs pairs (used for working TE modules) have to be also very low. This is another challenge, especially with Bi_2Te_3 and Sb_2Te_3 based materials that have generally a rough surface and need a conductive seed layer of different chemical composition. However, STO based films epitaxially grown by MBE have very low surface roughness and will not require seed layers, which is a favourable case. The remaining challenges with STO based TE films are (*i*) to effectively decrease the thermal conductivity by nanostructuration (and enhance the final figure of merit ZT), (*ii*) effectively grow *p*-type doped films, and (*iii*) build *p-n* legs pairs and micro TE modules with low contact resistances.

2. Research subject, work plan:

We propose to investigate, develop and enhance STO-based TE films grown by MBE, in the view to integrate it in *p-n* legs pairs and micro TE modules on Si. The main objectives of the PhD thesis will be to **(*i*)** effectively decrease the thermal conductivity by nanostructuration strategies, **(*ii*)** effectively grow *p*-type doped films, **(*iii*)** evaluate and decrease the interfacial contact resistances with electrodes, and **(*iv*)** develop technological tasks in the view to build *p-n* legs pairs and micro TE modules.
The first step (*i*) will be to optimize *n*-type La-doped STO films with optimal TE properties, by decreasing thermal conductivity through nanostructuration and atomic modulation strategies (by building short-period superlattices for instance) while maintaining large electrical conductivity and Seebeck coefficient by doping. **The second step (*ii*)** will be to

investigate a *p*-type dopant and grow optimized *p*-type doped STO films with large electrical conductivity and Seebeck coefficient. Once optimized, nanostructuration strategies will be applied in *p*-type doped films in order to decrease their thermal conductivity while maintaining large electrical conductivity and Seebeck coefficient. **The third step (*iii*)** will be to measure the interfacial contact electrical resistances between the developed TE materials and various conducting electrodes. Compatible electrodes with the lowest interfacial contact resistances will then be selected. **The fourth step (*iv*)** will be the evaluation of the easiest technological tasks to achieve the development of a micrometer thick *p*-*n* legs pair, to develop it and to measure its TE properties. If successful, the technological tasks will be extended to build an integrated micro TE module with various electrically-connected *p*-*n* legs pairs.

The PhD student will have to make the **elaboration** of the films, to **structurally and chemically characterize** them, and to **measure their full physical properties**. The growth of the STO based films with precise chemical composition and nanostructuration control at the atomic scale will be done by state-of-the-art oxide MBE available at ECL-INL. The structural properties will be measured by *in-situ* RHEED during growth, AFM and XRD. The chemical properties will be mainly measured by XPS, and also by TOF-SIMS and RBS through collaborations. The electrical conductivity will be measured by I-V curves. The charge carrier concentration and mobility will be measured by Hall effect in Van der Pauw geometry. The Seebeck measurements will be done in a home-made set-up. The thermal conductivity will be measured by SThM and 3ω technique (through collaborations). The interfacial contact resistances will be done by I-V curves with different electrodes (different materials and sizes). The technological steps will be realized at the NanoLyon platform hosted by ECL-INL.

3. References:

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