
SERB Fund for Industrial Research Engagement (SERB- FIRE)

Request for Proposal

The Scheme for funding Industry Relevant R&D (IRRD) of SERB aims to utilize the expertise available in academic institutions and national laboratories (“academic partners”) to solve industry specific problems for larger benefit of society. The Program titled ‘Fund for Industrial Research Engagement (FIRE)’ under IRRD supports ideas that address well-defined problems of industrial relevance in project mode. SERB signed partnership agreements with a few selected industries including Applied Materials India Private Limited (AMAT). Funding support by SERB and AMAT shall be on equal basis of 1:1 ratio for projects jointly executed by academic partners and AMAT under the program.

R&D proposals are solicited from scientists in specified themes. Following illustrations on the problem statement will guide the prospective investigators to align and sharpen their proposal. Accordingly, the Investigators are requested to go through the details carefully before submitting the proposal.

THRUST AREA

Atomically thin coatings enabled through Computational Modelling & deposition for Semiconductor & Pharma Applications and cytotoxicity studies of nanomaterials

PROBLEM DEFINITION/WORK SCOPE DEFINITION

Atomically Thin Coatings enabled through Molecular Modelling, Process control and characterization in the areas of Semiconductor & Life science applications.

PROBLEM ILLUSTRATION

The project should be centred around developing atomic layer deposition (ALD) techniques for specific application in the semiconductor and life science areas. Three key components of the project are computation – analysis to identify appropriate precursors, interaction mechanism between various aspect of the ALD process. Process – where the validation and the optimization activities will be carried out and the third is the characterization which will be a continuous feed to process optimisation as well as identifying key functionality of the coating. Overall, the expected output is the fundamental understanding of the ALD process and its outcome. Close interactions between the three aspects from PIs/participating institutes is an expectation with close interaction and contribution from Co-PI from Industry.

OBJECTIVES ANTICIPATED

Computationally accelerated material & process innovations on thin film-based coatings (Atomic Layer Deposition)

a) Modelling assisted precursor identification, reaction mechanisms and process development for thin film deposition (ALD) in the areas of semiconductor & life science applications.

- b) For Semiconductor applications the Material of interest (not limited to) are- metal oxides and metal nitrides, chalcogenides (-Interested class of metals M (III), M (IV), M (V)).
- c) For Life science applications molecular modelling study of nano coatings (inorganic) on organic particles
- d) Thermodynamic and kinetic study of reaction pathways, substrate-precursor interactions (surface reaction mechanism), preferential site preferences for selective deposition as well as computational predictive materials properties.
- e) Computational DFT modelling to predict ALD reaction mechanisms and potential precursors, synthetic route for precursor synthesis and ALD process development to evaluate the proposed chemistry on the ALD tool
- f) Process trials and development with identified precursors through modelling, validation of ALD coatings for semiconductor applications and process integration (Tech transfer & scale-up)
- g) Characterization for Semiconductor applications: Characterize the developed thin films (<20nm) with respect to thickness, surface roughness, morphology, and optical properties.
- h) Characterization for life science application:
 - a. Samples will be provided by AMAT
 - b. Establish toolbox for characterizing nano coating (<50nm) on organic particles and its interface leading to determination of film thickness, morphology chemical composition, stoichiometry, crystal structure, bonds, and coating thickness uniformity.

EXPECTED OUTPUT AND OUTCOME OF THE PROPOSAL

- Theoretical modelling should be able to recommend precursor to be used for ALD activities along with fundamentals based on thermodynamics and kinetics to recommend appropriate pathways. Eventually experimental data need to be provided to support the modelling outcomes.
- Modelling should also give an outcome of various possible reactions that will take place between substrate and precursors/ by-products/subsurface.
- The Characterization aspect should help in establishing techniques or combination of techniques that will provide the requisite information of the coating and its interface.

EXPECTATION FROM THE PI/INSTITUTION

- The PI/Co-PI should have carried out projects in the ALD domain and have a minimum of 5 years of experience in the domain
- PI/Co-PI should have ALD reactors (test reactor for small samples) that will support metal oxide and metal nitride film formation (-Interested class of metals M (III), M (IV), M (V))
 - Coating types: Metals, Oxides, Nitrides, Chalcogenides
- Reactor should be capable of handling organometallic precursors and/or halide precursors for metals and have appropriate abatement systems

- Relevant precursors forming above class of materials including mixed oxides, oxynitrides
- Core-shell architecture (Core-Oxides, non-oxides, organic compounds; shell-oxides, nitrides, chalcogenides etc)
- Participating institute should have required characterization tools for characterization of thin films (SEM/ TEM/ FIB/ XPS/ XRD/ XRR/ Ellipsometry/ AFM etc.)
- Computational projects to be led by PIs having a minimum 3 years of program management experience using DFT/Ab-initio for semiconductor application. Participating institute on such projects should have in-house capability for high performance computing and latest ab-initio package
- AMAT will have a Co-PI on the selected proposal
- AMAT will enter into MOU with the identified PI/institute once the proposal is selected

GENERAL GUIDELINES

- Applicants [Principal Investigator (PI) and Co-Principal Investigator(s) (Co-PI(s))] should be Indian citizens. The applicant(s) must hold a regular academic/research position in a recognized academic institution or national laboratory or in any other recognized R & D institution in India.
- The funding is provided for a period of two years. The research grant is provided for minor equipment (essential), manpower, consumables, travel and contingency. "Overheads" is also be provided to the implementing institution as per prevailing norms of SERB.
- All the rights, duties and obligations pertaining to any intellectual property, profit sharing/royalty and / or related aspects shall be discussed and agreed separately in writing with the participating academic institute(s) and AMAT under definitive agreement(s), in order to enable AMAT to commercialize and benefit from the developed solutions.

	AMAT	SERB
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Please visit SERB online portal for more details & submission of proposals.
(www.serbonline.in)