DARPA-EA-25-02-04
Crystal Substrate Bonding Technologies and Algorithms (CRYSTAL)

I. ARC Opportunity

The Defense Advanced Research Projects Agency (DARPA) Defense Sciences Office (DSO) is issuing an Advanced Research Concepts (ARC) Opportunity, inviting submissions of Abstracts for innovative exploratory research concepts in the technical domain of wafer bonding of thin-film crystals. This ARC Opportunity, Crystal Substrate Bonding Technologies and Algorithms (CRYSTAL), is issued under the master ARC Exploration Announcement (EA), DARPA-EA-25-02.

ARC Opportunities are designed to allow an individual researcher the opportunity and time to focus on nascent, paradigm-shifting ideas for national security applications. While multiple researchers from the same organization may be proposed, the aggregate level of effort for a proposed research concept are expected to be equivalent to one full-time equivalent (FTE) and 12 months as ARC topics are designed for ideas that nominally would take a full year effort (1 FTE over 1 year) to properly validate. DARPA expects that the individual(s) working on the proposed idea primarily focus on the effort for the entire period of performance to the maximum extent practical. The maximum period of performance is 12 months. Each ARC award's total cost should range from $100,000 to $300,000, including direct and indirect costs and graduate student tuition, if applicable. Proposed costs for materials, equipment, and Other Direct Costs (ODC) are limited as outlined in the master ARC EA, DARPA-EA-25-02. Under no circumstances will profit be authorized. While resource sharing is not expected, it may be offered in the proposal. DARPA understands not all ideas and organizations may fit in this parameter range and will work with a proposer to ensure truly innovative ideas can be explored with the required resources. Travel and publication costs may not be proposed. No subawardees are permitted.

To view the original DARPA Exploration Announcement and the latest amendment issued against Advanced Research Concepts, visit SAM.gov under solicitation number DARPA-EA-25-02: https://sam.gov/opp/95c31b3f3e094627a9a1e053766e46e1/view. It is incumbent upon the proposer to review DARPA-EA-25-02, any resulting amendments to DARPA-EA-25-02, and Frequently Asked Questions (FAQs) before preparing and submitting an Abstract and/or an Oral Proposal Package (OPP) (if invited). All Abstract submissions to this announcement must adhere to the instructions contained in DARPA EA-25-02.

All technical, contractual, and administrative questions regarding this notice must be emailed to CRYSTAL@darpa.mil. This ARC Opportunity is soliciting Abstracts only. DARPA will evaluate Abstracts submitted in response to this ARC Opportunity, as detailed in Section 4 of the latest amendment issued against DARPA-EA-25-02. If the Government selects an Abstract for an Oral Presentation, the Government will issue an invitation to submit an OPP. The invitation will include the submission instructions and deadline.

All awards made as a result of the ARC Opportunity will be Research Other Transactions (OTs) awarded under the authority of 10 U.S.C. § 4021.

Abstracts submitted to this ARC Opportunity will be evaluated on a rolling basis in accordance with the latest amendment issued against DARPA-EA-25-02. The end of the submission period will be 4:00 p.m. Eastern Time on June 16, 2025. No Abstracts will be accepted after the end of the submission period. Proposers are encouraged to submit Abstracts as early as possible. Funding for this ARC Opportunity is limited. Should funding be exhausted, the Government may elect to

shorten the overall submission period with an amendment to this ARC Opportunity.

II. ARC Opportunity Description

Bonded single crystal thin film multi-functional materials (electro-optic, acousto-electric, acousto-optic, magneto-optic or multi-ferroic materials) are vital for diverse sensing and communications technologies (integrated quantum, photonic, terahertz [THz], radio frequency [RF], and actuator platforms).[1] [2] Wafer bonding onto compatible substrates[3] is the critical step for integrating single crystal thin films into multi-functional devices and systems. There is currently no method to analytically investigate wafer bonding processes. Brute force experimentation is required for initial process development, and subsequent changes in materials or device parameters necessitate significant additional trial and error, incurring huge costs, prolonging timeframes, thus limiting exploration of novel material systems.

Because there are no generalizable approaches to model wafer bonding between thin film crystals and substrates, wafer bonding process development remains highly empirical. As a result, the wafer bonding process is highly specific to select materials and device parameters and is limited by experimental knowledge to a small subset of known materials and device parameters. As an example, although lithium niobate on insulator (LNOI) exhibits promising piezo-electric and electro-optic properties, the lack of predictive wafer bonding models impedes development of novel applications and limits scalable integration.[4] The ability to predictively model wafer bonding of thin film crystals would rapidly accelerate the research and development of multi-functional materials, and their fabrication and scalable integration in diverse applications.

This ARC Opportunity is soliciting ideas to explore the following question:

To accelerate development and integration of multi-functional materials, how do we create generalizable models to explore thin film crystal bonding onto suitable substrates under diverse real-world process conditions and parameters?

A. ARC Opportunity Technical Objective

CRYSTAL aims to investigate fundamental modeling frameworks for bonding thin film crystalline multi-functional materials onto compatible substrates under diverse process conditions. The target outcome is the creation of modeling frameworks for wafer fabrication and bonding, which capture interface properties and material-substrate compatibility, and enable reliable prediction of optimal wafer bonding conditions designed to meet desired material and device design parameters. Successful models developed under this solicitation will enable accelerated discovery, design, and fabrication of novel bonded single crystal thin-film material systems.

The material design parameters for consideration include, but are not limited to: thin film

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[1] Boes, Andreas, et al. "Lithium niobate photonics: Unlocking the electromagnetic spectrum." *Science* 379.6627 (2023): eabj4396.
[2] Castelletto, Stefania, et al. "Silicon carbide photonics bridging quantum technology." *ACS Photonics* 9.5 (2022): 1434-1457.
[3] Gösele, U., and Q-Y. Tong. "Semiconductor wafer bonding." *Annual review of materials science* 28.1 (1998): 215-241.
[4] Mookherjea, Shayan, Viphretuo Mere, and Forrest Valdez. "Thin-film lithium niobate electro-optic modulators: to etch or not to etch." *Applied Physics Letters* 122.12 (2023).

thickness, crystal orientation, surface preparation, oxide thickness, substrate material, and wafer size. The target device fabrication and interface formation conditions from the developed model should include, but are not limited to: bonding temperature, bonding pressure, ion implantation dose, time, and gradients and transients of temperature and pressure.

The CRYSTAL ARC Opportunity seeks proposals that dramatically increase the understanding of thin film crystal-substrate wafer bonding through a modeling/simulation framework. Material-substrate platforms that have been extensively studied (e.g., silicon on insulator) or cannot be bonded with variable thin film thickness (e.g., graphene or N-doped carbon) are out of scope. This ARC Opportunity asks proposers to do this through the following process:

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- Model development: Create a bonding model for a material-substrate platform of the proposer's choice which exhibits multi-functional properties. Further, justify how the model framework should be applicable for any wafer design parameters and compatible substrates. Development of the model should be guided by experimental results (e.g., preliminary data or gathered from published literature), as per guidance in Section II.B.

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- Model assessment: First, test model applicability on LNOI bonding for assessing the feasibility of fabricating commercially available LNOI wafers either in simulation, or by comparing against known material properties and/or recipes of the proposer's choice. Second, repeat assessment for any one of the following thin film crystals bonded to substrate: lithium tantalate on insulator, silicon carbide on insulator, yttrium iron garnet on insulator, or gallium nitride on any substrate. Model assessment is not expected to include significant additional model development.

Model development is the first step of the process. Government acceptance of completed model development is a requirement for proceeding with model assessment.

The primary modeling component should involve multi-physics interface modeling which incorporates real-world process conditions (e.g., gradients of temperature and pressure, ion implantation dose, etc.). Potential approaches could combine surface chemistry modeling, molecular dynamics, finite-element methods, analytical methods, and/or other appropriate modeling techniques. The target model should quantify the effects of process parameters (e.g., temperature, pressure, ion implantation dose, time, and gradients and transients of temperature and pressure) on the crystal-substrate bonding phenomena. Additionally, any significant change in material properties due to variation of bonding formation conditions should be explored.

B. ARC Abstracts

CRYSTAL ARC abstract submissions must provide a substantial technical description of the proposed approach that will be investigated in exploring the physical and chemical processes that govern crystal-substrate bonding phenomena. For model development, abstracts must describe the proposed multi-functional material and substrate, and explain potential applications. Abstracts must provide a technical description of the computational approach for modeling crystal-substrate interface formation and material properties, provide evidence for why the approach has merit, and explain how the approach can be generalized to arbitrary substrates. Abstracts should describe how experimentally gathered results (preliminary data or published literature) will be used to guide the development of the proposed computational models, and should specify the source(s) of the

experimental data.

Abstracts should clearly explain how the proposed modeling approach addresses fundamental limitations and technical gaps. Abstracts should also include a detailed research plan that includes: (1) detailed intermediate technical objectives with evaluation measures; and (2) a schedule segmented monthly and quarterly outlining corresponding deliverables. Approaches that do not significantly advance the state of the art may be considered out of scope.

This ARC Opportunity is intended to be as inclusive as possible; however, proposed ideas should address the appropriate scope, have a clear deliverable at the end of the effort, and include specific practical applications of the research.

We highly encourage submitters with or without prior Department of Defense related research experience to apply for this opportunity.

DARPA will evaluate Abstracts submitted in response to this ARC Opportunity, as detailed in Section 4 of the latest amendment issued against DARPA-EA-25-02. If the Government selects an Abstract for an Oral Presentation, the Government will issue an invitation to submit an OPP. The invitation will include the submission instructions and deadline.

C. Schedule of Milestones

The specific milestones and due dates listed are common to all Abstracts and OPPs (see above for technical details and Section III.A below for additional information on milestones). Abstracts selected to submit an OPP will be required to propose milestones associated with the program plan as part of the oral proposal.

- Kick-off meeting: Should define the technical approach and steps forward.
- Milestone status meetings: Briefing to include detailed progress towards all research objectives, progress to plan, and discussion of next milestone objectives.
- Final Opportunity outbrief: The final briefing should summarize all work completed on the project.

D. Reporting Requirements

Performers will be expected to provide at a minimum the following reports:

- Monthly update reports: These technical and financial reports should include progress to plan.
- Milestone technical report: Each report should detail progress towards all research objectives and should include a master document that refers to associated explanatory presentation slides, models, modeling data and results, model verification data, and software source code with full documentation, as needed.
- Model development report: This report should be submitted at completion of Model development, and must include explanatory presentation slides, algorithms, models, modeling data and results, and software source code with full documentation.
- Model assessment report: This report should be submitted at completion of assessment, and must include model assessment data, algorithms and source code, and explanatory slides comparing data from the model with experimental data.
- Final technical report: The final report should include the final master document from the Milestone technical reports, Model development report and Model assessment report, and

detail results of all milestones associated with the program plan for the entire period of performance. The final and all intermediate algorithms, models, modeling data and results, model assessment data, and software source code with full documentation should also be included.

III. ARC Opportunity Submission Format, Instructions and Selection

A. Abstract Content and Format

All Abstracts submitted in response to this notice must comply with the content and format instructions in Section 3.1 of the latest amendment issued against DARPA-EA-25-02. The submission must use the template provided as attachment to DARPA-EA-25-02. Abstracts submitted in response to this ARC Opportunity must be unclassified.

B. Abstract and OPP Submission Instructions

Abstracts submitted in response to this ARC Opportunity and OPPs submitted in response to an invitation shall be submitted electronically via the DARPA Submission website at https://baa.darpa.mil. See Section 3.3 of the latest amendment issued against DARPA-EA-25-02 for Abstract and OPP submission instructions.

Technical support for the DARPA Submission website is available during regular business hours, Monday – Friday, 9:00 a.m. – 5:00 p.m. Eastern Time. Requests for technical support must be emailed to BAAT_Support@darpa.mil with a copy to CRYSTAL@darpa.mil. Questions regarding submission contents, format, deadlines, etc. should be emailed to CRYSTAL@darpa.mil. Questions/requests for support sent to any other email address may result in delayed/no response.

DARPA will acknowledge receipt of complete submissions via email and assign identifying numbers that should be used in all further correspondence regarding those submissions. If no confirmation is received within two (2) business days, please contact CRYSTAL@darpa.mil to verify receipt.

No Abstracts will be accepted after the end of the overall submission period listed in Section I above. Abstracts must be submitted per the instructions outlined in this ARC Opportunity *and received by DARPA* no later than this time and date. Proposers are advised that the Abstract submission deadline outlined herein is in Eastern Time.

Abstracts will be evaluated and selected in accordance with Section 4 of the latest amendment issued against DARPA-EA-25-02.

IV. Award Information

Selected OPPs will result in a potential award of a Research OT agreement subject to the proposer's acceptance of the terms and conditions. Proposers must review the model Research OT agreement provided as Attachment E to DARPA-EA-25-02.

The completed Task Description Document, Schedule of Milestones and Payments (templates included in Attachment E), and data rights will be included in the Research OT agreement upon award.

Given the limited funding available for each ARC Opportunity, not all proposals considered selectable may be selected for a potential award.

V. Eligibility

See Section 6 of the latest amendment issued against DARPA-EA-25-02 for information on who may be eligible to respond to this notice.

VI. Human Subject Research

Abstracts to this ARC Opportunity proposing human subjects research will be considered out of scope and may be disregarded.

VII. Administrative Requirements

Section 7.2 of the latest amendment issued against DARPA-EA-25-02 provides information on administrative requirements that may be applicable for proposal submission as well as performance under an award.

VIII. Frequently Asked Questions (FAQs)

All technical, contractual, and administrative questions regarding this notice must be emailed to CRYSTAL@darpa.mil. Emails sent directly to the ARC Manager or any other address may result in delayed or no response.

All questions must be in English and must include the name, email address, and telephone number of a point of contact. DARPA will attempt to answer questions publicly in a timely manner; however, questions submitted within seven (7) calendar days of the proposal due date listed herein may not be answered.

DARPA may post an FAQ list under the CRYSTAL ARC Opportunity on the DARPA website, http://www.darpa.mil. The list will be updated on an ongoing basis until one (1) week prior to the abstract due date. DARPA will also maintain https://www.darpa.mil/ARC as a resource page with links to all relevant ARC Opportunities and FAQs.