

**METAL CHALCOGENIDE NANOSTRUCTURED
MATERIALS FOR THEIR IMPROVED
THERMOELECTRIC AND
MECHANICAL PERFORMANCE**

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by

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Submitted

in fulfilment of the requirement of the degree of Doctor of Philosophy
to the



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CERTIFICATE

This is to certify that the thesis entitled “**Metal Chalcogenide Nanostructured Materials for Their Improved Thermoelectric and Mechanical Performance,**” submitted by **Mr. Jamal Ahmad Khan** to the Indian Institute of Technology Delhi, is worthy of consideration for the award of the degree of **Doctor of Philosophy** and is a Bonafide record of the research work carried out by him under my supervision. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

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DEDICATED TO MY PARENTS

ABSTRACT

The global warming and the alarming rate of carbon emissions has led to the increase of the earth's temperature by 1°C. The fossil fuel combustion generates about 90% of the global energy with an efficiency of 30-40% and the rest is turned into waste heat. Thus, there is an immediate need to restrain alarming emissions of carbon and provide a feasible solution for waste heat management. In order to circumvent this energy wastage, immense efforts need to be devoted towards sustainable and green energy solutions. Thermoelectric (TE) technology has been a promising solution to meet the inevitable global energy demands, which enables the direct conversion of thermal energy into electricity and vice versa. Increasing the thermoelectric figure of merit of thermoelectric materials is of prime importance in order to realize their practical applications. An efficient TE material must have high power factor ($S^2\sigma$) and minimum thermal conductivity (κ). However, owing to the conflicting dependence of the factors governing zT , it is a challenging task to attain maximum possible zT . In addition, the brittle nature of these materials creates constraint in the fabrication of flexible thermoelectric devices.

The above background forms the basis of objectives of the present work. The central objective of the thesis is to explore the various strategies for improving the thermoelectric performance of Metal Chalcogenides and investigating their nanomechanical response. Further, this thesis has employed a diverse range of experimental approaches, including electrical, and thermoelectric measurements, as well as theoretical methods such as DFT calculations, to offer these valuable insights. While analyzing the properties of as-prepared thermoelectric materials, this thesis presents the different mechanical studies of nanostructured materials and their effect on mechanical properties of nanocomposites. The mechanical properties of Zinc gallium oxide ($ZnGa_2O_4$) nanostructures and Ag nanorods treated Kevlar composites is also discussed using various mechanical testing systems.

In the first section of the work, we fabricated the Ag_2Se nanorod arrays and ordinary thin films on the glass substrates by glancing angle deposition technique (GLAD) followed by selenization in a two-zone furnace. The unique tilted Ag_2Se nanorod arrays shows a excellent $zT = 1.14 \pm 0.09$ and power factor of $3229.21 \pm 149.01 \mu W/m-K^2$, respectively at 300 K. The superior thermoelectric performance of Ag_2Se nanorod arrays compared to planar Ag_2Se films could be ascribed to the unique nanocolumnar architecture that not only

facilitates efficient electron transport but also significantly scatter phonons at the interfaces. the nanoindentation measurements were performed to explore mechanical properties of the as-prepared films. The Ag₂Se nanorod arrays showed hardness values of 116.51 ± 4.25 MPa and elastic modulus of $10,966.01 \pm 529.61$ MPa, which are lowered by 51.8 % and 45.6 %, compared to Ag₂Se films, respectively.

In addition to tilted and straight wire morphology, it is interesting to investigate nanostructures of complex morphologies for improved TE properties. In this regard, the zig-zag Ag₂Se nanorod arrays were prepared on the glass substrates by glancing angle deposition technique (GLAD) followed by selenization in a two-zone furnace. A high zT value of 1.29 ± 0.31 at room temperature in the hierarchical zig-zag Ag₂Se nanorod arrays fabricated using Glancing angle deposition technique (GLAD) followed by a facile selenization process. The high zT value at 300 K is ascribed to the ultrahigh power factor of $3101 \pm 252 \mu\text{W/m}\cdot\text{K}^2$ and the reduced thermal conductivity of 0.72 ± 0.01 W/mK. Based on *ab initio* computational and experimental evidence, we reveal that kinked Ag₂Se nanorod arrays consisting of rough interfaces modulate the lattice thermal conductivity up to 48.5% at room temperature. The modulation results from interchanging of phonon modes at kink points and enhanced scattering from large number of rough interfaces. Further, benefitting from kinked hierarchy, a notable improvement in the mechanical performance is observed for zig-zag Ag₂Se nanorods which is confirmed by nanoindentation measurements. The compliant architecture of multiple armed zig-zag Ag₂Se nanorod arrays makes them less prone to damage and fracture compared to single arm Ag₂Se nanorods, thereby improving their elastic properties which is favourable for the fabrication of flexible TE devices.

Large-scale research is being done for the preparation of conducting polymer- and Ag₂Se-based organic composites for flexible TE devices. However, the performance of these hybrid materials could not compete with their inorganic counterpart. In this regard, we prepared a series of polycrystalline Ag₂Se_{1-x}S_x ($x = 0.00, 0.15, 0.20, 0.25$ and 0.30) samples were via melting approach. The correlation between their crystalline structures, TE properties and mechanical performance were systematically investigated. The sulfur alloyed samples exhibit the formation of highly crystallized grains that would positively favour electrical conductivity. Meanwhile, the presence of defects such as stacking faults, dislocations, twin boundaries and grain boundaries not only contributes to the reduction in

lattice thermal conductivity but also improves the elastic behaviour of the sulfur alloyed Ag_2Se samples. In addition, the formation of distinct diffraction spots and amorphous rings were observed in SAED pattern, that confirms the coexistence of crystalline and amorphous phase. Further, the mechanical and viscoelastic properties were examined via dynamic mechanical analysis using nanoindentation. The viscoelastic properties involve measurement of storage modulus (E'), loss modulus (E'') and $\tan \delta$ as a function of penetration depth. Intriguingly, for all samples a corresponding lower value of E'' is observed compared to E' values, representing a typical viscoelastic behaviour of the $\text{Ag}_2\text{Se}_{1-x}\text{S}_x$ system. The decreasing trend in the E' values is attributed to the unique crystal structure of the monoclinic $\alpha\text{-Ag}_2\text{S}$ grains that are formed with increasing S content. This study provides the opportunity to simultaneously tailor the TE and mechanical properties of Ag_2Se by suitable sulfur concentration.

Among various approaches towards improving the thermoelectric response, hot carrier filtering is one of the most promising one. The central objective of this work is to demonstrate the hot carrier filtering effect as a means to improve the thermoelectric properties of the SnTe-Au nanocomposite samples. Au nanoparticles grown via electrochemical deposition are incorporated in SnTe thin films prepared by RF magnetron sputtering. Thermoelectric properties have been investigated as a function of Au nanoparticles concentration. An optimal value of 0.8 atomic % Au NPs concentration with 40 nm size leads to a substantial improvement in TE response, specifically in terms of power factor. The achieved power factor value of $55.08 \mu\text{W}/\text{cm}\cdot\text{K}^2$ at 500 K is 66.4% improved compared to power factor values from pristine SnTe sample. The results indicate that controlling and optimizing the concentration of Au NPs is crucial in order to reduce the impact of negative charge carriers. A significant finding of this work is that a departure from a certain carrier concentration could significantly diminish the advantages gained from the carrier filtering method.

Aramid fibers, like Kevlar, have the highest specific toughness and strength of any commercially available fiber, making them ideal for soft body armor and reinforcing fibers in ballistic composite laminates. However, for better protection, the ballistic resistance of soft body armor should be improved, and the inert surface of aramid fibers generates low interfacial shear strength, resulting in inferior mechanical properties of composites. Controlling the surface/interphase properties of the fibers is thus required to both tune the

inter-yarn friction, which improves the soft body armor's ballistic performance, and the composite's properties. This work reports the fabrication of aligned silver (Ag) nanorods on para-aramid (Kevlar) fiber surfaces using a unique glancing angle deposition technique aimed at enhancing inter-yarn friction. The study investigates the influence of Ag nanorods on the mechanical properties of Kevlar-epoxy composites under diverse loading conditions. The tensile and flexural strength of Kevlar epoxy composites increased by 13.2% and 39.8%, respectively, after coating of Ag nanorods on the Kevlar fabric surface. Meanwhile, the Impact energy absorption by Kevlar epoxy composites was improved dramatically after the development of Ag nanorods on the Kevlar fabric surface. The impact tests were further validated by finite element analysis using Ansys software. The results show promise for the use of Ag nanorods interfaced Kevlar composites for impact resistance applications.

The ultrawide bandgap, high fields stability and robustness make ZnGa_2O_4 be an excellent candidate for devices like photodetectors, light-emitting diodes operating in deep ultraviolet wavelength regimes and power devices application. Keeping in mind the vivid potential applications of the ZnGa_2O_4 ceramics, investigation of the mechanical properties of the ZnGa_2O_4 spinel is important. The role of sintering on the microstructure and mechanical properties of ZnGa_2O_4 pellets has been systematically investigated in this work. The Hardness (H) and elastic modulus (E) of the sintered pellets were obtained via quasi-static and dynamic nanoindentation. The force versus displacement curves revealed the elastic-plastic behaviour of the ZnGa_2O_4 ceramics. The H and E values of the sintered pellets vary within 5.29-3.94 GPa and 149.25 -111.04 GPa, respectively. A decreasing trend is observed in both H and E of the sintered pellets with increased sintering duration, which could be ascribed to the grain size of the sintered products. The results from the dynamic nanoindentation testing reveal that ZnGa_2O_4 ceramics show a reverse indentation size effect (RISE). In addition, the viscoelastic properties of the sintered ZnGa_2O_4 ceramics were examined via dynamic nanoindentation. A higher storage modulus of 121 GPa with a corresponding low damping factor was obtained.

सारांश

ग्लोबल वार्मिंग और कार्बन उत्सर्जन की खतरनाक दर के कारण पृथ्वी के तापमान में 1 डिग्री सेल्सियस की वृद्धि हुई है। जीवाश्म ईंधन दहन 30-40% की दक्षता के साथ वैश्विक ऊर्जा का लगभग 90% उत्पन्न करता है और बाकी अपशिष्ट गर्मी में बदल जाता है। इस प्रकार, कार्बन के खतरनाक उत्सर्जन को रोकने और अपशिष्ट ताप प्रबंधन के लिए एक व्यवहार्य समाधान प्रदान करने की तत्काल आवश्यकता है। इस ऊर्जा की बर्बादी को रोकने के लिए, स्थायी और हरित ऊर्जा समाधानों की दिशा में अपार प्रयास किए जाने की आवश्यकता है। थर्मोइलेक्ट्रिक (टीई) प्रौद्योगिकी अपरिहार्य वैश्विक ऊर्जा मांगों को पूरा करने के लिए एक आशाजनक समाधान रही है, जो तापीय ऊर्जा को बिजली में सीधे परिवर्तित करने में सक्षम बनाती है। उनके व्यावहारिक अनुप्रयोगों को साकार करने के लिए थर्मोइलेक्ट्रिक सामग्रियों की योग्यता के थर्मोइलेक्ट्रिक आंकड़े को बढ़ाना प्रमुख महत्व का है। एक कुशल टीई सामग्री में उच्च शक्ति कारक ($S^2\sigma$) और न्यूनतम तापीय चालकता (κ) होनी चाहिए। हालांकि, जेडटी को नियंत्रित करने वाले कारकों की परस्पर विरोधी निर्भरता के कारण, अधिकतम संभव जेडटी प्राप्त करना एक चुनौतीपूर्ण कार्य है। इसके अलावा, इन सामग्रियों की भंगुर प्रकृति लचीले थर्मोइलेक्ट्रिक उपकरणों के निर्माण में बाधा पैदा करती है।

उपरोक्त पृष्ठभूमि वर्तमान कार्य के उद्देश्यों का आधार है। थीसिस का केंद्रीय उद्देश्य धातु चालकोजेनाइड्स के थर्मोइलेक्ट्रिक प्रदर्शन में सुधार के लिए विभिन्न रणनीतियों का पता लगाना और उनकी नैनोमैकेनिकल प्रतिक्रिया की जांच करना है। इसके अलावा, इस थीसिस ने इन मूल्यवान अंतर्दृष्टि प्रदान करने के लिए विद्युत और थर्मोइलेक्ट्रिक मापों के साथ-साथ डी. एफ. टी. गणना जैसे सैद्धांतिक तरीकों सहित विभिन्न प्रकार के प्रयोगात्मक तरीकों को नियोजित किया है। तैयार थर्मोइलेक्ट्रिक सामग्रियों के गुणों का विश्लेषण करते समय, यह थीसिस नैनोस्ट्रक्चर्ड सामग्रियों के विभिन्न यांत्रिक अध्ययनों और नैनोकंपोजिट्स के यांत्रिक गुणों पर उनके प्रभाव को प्रस्तुत करता है। जिंक गैलियम ऑक्साइड ($ZnGa_2O_4$) नैनोस्ट्रक्चर और एजी नैनोरोड उपचारित केवलर कंपोजिट के यांत्रिक गुणों पर भी विभिन्न यांत्रिक परीक्षण प्रणालियों का उपयोग करके चर्चा की जाती है।

काम के पहले खंड में, हमने ग्लैसिंग एंगल डिपोजिशन तकनीक (GLAD) द्वारा ग्लास सबस्ट्रेट पर Ag_2Se नैनोरोड सरणी और साधारण पतली फिल्मों का निर्माण किया, जिसके बाद दो-ज़ोन भट्टी में सेलेनाइजेशन किया गया। अद्वितीय झुकी हुई Ag_2Se नैनोरोड सरणी एक उत्कृष्ट $zT = 1.14 \pm 0.09$ और $3229.21 \pm 149.01 \mu W/m-K^2$ का पावर फैक्टर दिखाती है, जो क्रमशः 300 K पर है। प्लेनर Ag_2Se फिल्मों की तुलना में Ag_2Se नैनोरोड सरणी के बेहतर थर्मोइलेक्ट्रिक प्रदर्शन को अद्वितीय नैनोक्लमर वास्तुकला के लिए जिम्मेदार ठहराया जा सकता है जो न केवल कुशल इलेक्ट्रॉन परिवहन

की सुविधा प्रदान करता है बल्कि इंटरफेस पर फोनोन को भी महत्वपूर्ण रूप से बिखेरता है। तैयार फिल्मों के यांत्रिक गुणों का पता लगाने के लिए नैनोइंडेंटेशन माप किए गए थे। Ag_2Se नैनोरोड सरणी ने 116.51 ± 4.25 MPa की कठोरता मान और $10,966.01 \pm 529.61$ MPa के लोचदार मापांक दिखाए, जो क्रमशः Ag_2Se फिल्मों की तुलना में 51.8% और 45.6% कम हैं। झुका हुआ और सीधा तार आकृति विज्ञान के अलावा, बेहतर टीई गुणों के लिए जटिल आकृति विज्ञान के नैनोस्ट्रक्चर की जांच करना दिलचस्प है। इस संबंध में, ज़िग-ज़ैग Ag_2Se नैनोरोड सरणी को ग्लास सबस्ट्रेट्स पर ग्लैसिंग एंगल डिपोजिशन तकनीक (GLAD) द्वारा तैयार किया गया था, जिसके बाद दो-ज़ोन भट्टी में सेलेनाइजेशन किया गया था। श्रेणीबद्ध ज़िग-ज़ैग Ag_2Se नैनोरोड सरणी में कमरे के तापमान पर 1.29 ± 0.31 का एक उच्च zT मान ग्लैसिंग एंगल डिपोजिशन तकनीक (GLAD) का उपयोग करके गढ़ा गया है, जिसके बाद एक आसान सेलेनाइजेशन प्रक्रिया होती है। 300 K पर उच्च zT मान $3101 \pm 252 \mu W/m \cdot K^2$ के अल्ट्राहाइ पावर फैक्टर और 0.72 ± 0.01 W/mK की कम थर्मल चालकता के लिए जिम्मेदार है। *ab initio* कम्प्यूटेशनल और प्रयोगात्मक साक्ष्य के आधार पर, हम बताते हैं कि किंक किए गए Ag_2Se नैनोरोड सरणियों में रफ इंटरफेस होते हैं जो कमरे के तापमान पर 48.5% तक जाली थर्मल चालकता को संशोधित करते हैं। मॉड्यूलेशन किंक बिंदुओं पर फोनॉन मोड के आदान-प्रदान और बड़ी संख्या में रफ इंटरफेस से बढ़े हुए प्रकीर्णन के परिणामस्वरूप होता है। इसके अलावा, किंक पदानुक्रम से लाभान्वित होकर, ज़िग-ज़ैग Ag_2Se नैनोरोड्स के लिए यांत्रिक प्रदर्शन में एक उल्लेखनीय सुधार देखा गया है जिसकी पुष्टि नैनोइंडेंटेशन माप द्वारा की जाती है। कई सशस्त्र ज़िग-ज़ैग Ag_2Se नैनोरोड सरणियों की अनुरूप वास्तुकला उन्हें एकल भुजा Ag_2Se नैनोरोड की तुलना में नुकसान और फ्रैक्चर के लिए कम प्रवण बनाती है, जिससे उनके लोचदार गुणों में सुधार होता है जो लचीले TE उपकरणों के निर्माण के लिए अनुकूल है।

लचीले टीई उपकरणों के लिए पॉलिमर-और एजी2सी-आधारित कार्बनिक यौगिकों के संचालन की तैयारी के लिए बड़े पैमाने पर शोध किया जा रहा है। हालाँकि, इन संकर पदार्थों का प्रदर्शन उनके अकार्बनिक समकक्ष के साथ प्रतिस्पर्धा नहीं कर सका। इस संबंध में, हमने पॉलीक्रिस्टलाइन $Ag_2Se_{1-x}S_x$ ($x = 0.00, 0.15, 0.20, 0.25$ और 0.30) नमूनों की एक श्रृंखला तैयार की, जो पिघलने के दृष्टिकोण के माध्यम से थे। उनकी क्रिस्टलीय संरचनाओं, टीई गुणों और यांत्रिक प्रदर्शन के बीच सहसंबंध की व्यवस्थित रूप से जांच की गई थी। सल्फर मिश्र धातु के नमूने अत्यधिक क्रिस्टलीकृत कणों के गठन को प्रदर्शित करते हैं जो सकारात्मक रूप से विद्युत चालकता का समर्थन करेंगे। इस बीच, स्टैकिंग फॉल्ट, डिसलोकेशन, ट्विन बाउंड्री और ग्रेन बाउंड्री जैसे दोषों की उपस्थिति न केवल जाली थर्मल चालकता में कमी में योगदान देती है, बल्कि सल्फर मिश्र धातु Ag_2Se नमूनों के लोचदार व्यवहार में भी सुधार करती है। इसके अलावा, एसएईडी पैटर्न में अलग-अलग विवर्तन धब्बे और अनाकार वलय

का गठन देखा गया, जो क्रिस्टलीय और अनाकार चरण के सह-अस्तित्व की पुष्टि करता है। इसके अलावा, नैनोइंडेंटेशन का उपयोग करके गतिशील यांत्रिक विश्लेषण के माध्यम से यांत्रिक और विस्कोलास्टिक गुणों की जांच की गई। विस्कोइलास्टिक गुणों में भंडारण मापांक (ई') हानि मापांक (ई'') और टैन δ को प्रवेश गहराई के कार्य के रूप में मापना शामिल है। दिलचस्प रूप से, सभी नमूनों के लिए E' मानों की तुलना में E'' का एक संबंधित कम मान देखा जाता है, जो $Ag_2Se_{1-x}S_x$ प्रणाली के एक विशिष्ट विस्कोलास्टिक व्यवहार का प्रतिनिधित्व करता है। ई' मानों में घटती प्रवृत्ति का श्रेय मोनोक्लिनिक $\alpha-Ag_2S$ अनाज की अनूठी क्रिस्टल संरचना को दिया जाता है जो बढ़ती एस सामग्री के साथ बनती हैं। यह अध्ययन उपयुक्त सल्फर सांद्रता द्वारा Ag_2Se के TE और यांत्रिक गुणों को एक साथ तैयार करने का अवसर प्रदान करता है।

थर्मोइलेक्ट्रिक प्रतिक्रिया में सुधार की दिशा में विभिन्न दृष्टिकोण के बीच, गर्म वाहक फ़िल्टरिंग सबसे आशाजनक है। इस कार्य का केंद्रीय उद्देश्य एसएनटीई-एयू नैनोकम्पोजिट नमूनों के थर्मोइलेक्ट्रिक गुणों में सुधार के साधन के रूप में गर्म वाहक फ़िल्टरिंग प्रभाव को प्रदर्शित करना है। विद्युत रासायनिक निक्षेपण के माध्यम से उगाए गए एयू नैनोकणों को आरएफ मैग्नेट्रॉन स्पटरिंग द्वारा तैयार एसएनटीई पतली फिल्मों में शामिल किया जाता है। औ नैनोकणों की सांद्रता के एक कार्य के रूप में ऊष्मीय-विद्युत गुणों की जांच की गई है। 40 एनएम आकार के साथ 0.8 परमाणु% एयू एनपीएस सांद्रता का एक इष्टतम मूल्य टीई प्रतिक्रिया में पर्याप्त सुधार की ओर ले जाता है, विशेष रूप से पावर फैक्टर के संदर्भ में। 500 K पर $55.08 \mu W/cm-K^2$ का प्राप्त पावर फैक्टर (power factor) मूल्य 66.4% है जो प्राचीन SnTe नमूने से पावर फैक्टर (power factor) मूल्यों की तुलना में बेहतर है। परिणाम इंगित करते हैं कि नकारात्मक चार्ज वाहकों के प्रभाव को कम करने के लिए एयू एनपी की सांद्रता को नियंत्रित करना और अनुकूलित करना महत्वपूर्ण है। इस काम की एक महत्वपूर्ण खोज यह है कि एक निश्चित वाहक एकाग्रता से प्रस्थान वाहक फ़िल्टरिंग विधि से प्राप्त लाभों को काफी कम कर सकता है।

केवलर जैसे अरामिड फाइबर में किसी भी व्यावसायिक रूप से उपलब्ध फाइबर की उच्चतम विशिष्ट कठोरता और ताकत होती है, जो उन्हें नरम शरीर कवच और बैलिस्टिक समग्र लैमिनेट्स में फाइबर को मजबूत करने के लिए आदर्श बनाती है। हालांकि, बेहतर सुरक्षा के लिए, नरम शरीर कवच के बैलिस्टिक प्रतिरोध में सुधार किया जाना चाहिए, और अरामिड फाइबर की निष्क्रिय सतह कम अंतरफलक कतरनी शक्ति उत्पन्न करती है, जिसके परिणामस्वरूप कंपोजिट के निम्न यांत्रिक गुण होते हैं। इस प्रकार रेशों की सतह/अंतर-चरण गुणों को नियंत्रित करने के लिए अंतर-सूत घर्षण दोनों को ट्यून करने की आवश्यकता होती है, जो नरम शरीर कवच के बैलिस्टिक प्रदर्शन और समग्र के गुणों में सुधार करता है। यह काम पैरा-अरामिड (केवलर) फाइबर सतहों पर सरेखित सिल्वर (एजी)

नैनोरोड्स के निर्माण की रिपोर्ट करता है, जिसका उद्देश्य अंतर-धागे के घर्षण को बढ़ाना है। अध्ययन विविध लोडिंग परिस्थितियों में केवलर-इपोक्सी कंपोजिट के यांत्रिक गुणों पर एजी नैनोरोड के प्रभाव की जांच करता है। केवलर कपड़े की सतह पर Ag नैनोरोड्स की कोटिंग के बाद केवलर एपॉक्सी कंपोजिट की तन्यता और लचीलापन क्रमशः 13.2% और 39.8% बढ़ गया। इस बीच, केवलर कपड़े की सतह पर एजी नैनोरोड के विकास के बाद केवलर एपॉक्सी कंपोजिट द्वारा प्रभाव ऊर्जा अवशोषण में नाटकीय रूप से सुधार हुआ। प्रभाव परीक्षणों को आगे एंसिस सॉफ्टवेयर का उपयोग करके परिमित तत्व विश्लेषण द्वारा मान्य किया गया था। परिणाम प्रभाव प्रतिरोध अनुप्रयोगों के लिए एजी नैनोरोड्स इंटरफेस केवलर कंपोजिट के उपयोग के लिए वादा दिखाते हैं।

अल्ट्रावाइड बैंडगैप, उच्च क्षेत्र स्थिरता और मजबूती $ZnGa_2O_4$ को फोटोडिटेक्टर, गहरे पराबैंगनी तरंग दैर्ध्य शासन और बिजली उपकरणों के अनुप्रयोग में काम करने वाले प्रकाश उत्सर्जक डायोड जैसे उपकरणों के लिए एक उत्कृष्ट उम्मीदवार बनाती है। $ZnGa_2O_4$ चीनी मिट्टी के बर्तनों के जीवंत संभावित अनुप्रयोगों को ध्यान में रखते हुए, $ZnGa_2O_4$ स्पिनल के यांत्रिक गुणों की जांच महत्वपूर्ण है। इस कार्य में $ZnGa_2O_4$ छरों के सूक्ष्म संरचना और यांत्रिक गुणों पर सिंटरिंग की भूमिका की व्यवस्थित रूप से जांच की गई है। सिंटर किए गए छरों की कठोरता (एच) और लोचदार मापांक (ई) अर्ध-स्थिर और गतिशील नैनोइंडेंटेशन के माध्यम से प्राप्त किए गए थे। बल बनाम विस्थापन वक्रों ने $ZnGa_2O_4$ चीनी मिट्टी के बर्तनों के लोचदार-प्लास्टिक व्यवहार को प्रकट किया। सिंटर किए गए छरों के एच और ई मान क्रमशः 5.29-3.94 जीपीए और 149.25-111.04 जीपीए के भीतर भिन्न होते हैं। सिंटरिंग अवधि में वृद्धि के साथ सिंटर छरों के एच और ई दोनों में एक घटती प्रवृत्ति देखी गई है, जिसे सिंटर उत्पादों के अनाज के आकार के लिए जिम्मेदार ठहराया जा सकता है। डायनेमिक नैनोइंडेंटेशन परीक्षण के परिणामों से पता चलता है कि $ZnGa_2O_4$ सिरामिक एक रिवर्स इंडेंटेशन आकार प्रभाव दिखाते हैं (RISE). इसके अलावा, सिंटर किए गए $ZnGa_2O_4$ सिरामिक के विस्कोलास्टिक गुणों की जांच गतिशील नैनोइंडेंटेशन के माध्यम से की गई थी। 121 जी. पी. ए. का एक उच्च भंडारण मापांक एक संबंधित कम अवमंदन कारक के साथ प्राप्त किया गया था।

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NOMENCLATURE

List of Symbols

ΔV	Potential difference
ΔT	Temperature difference
S	Seebeck coefficient
σ	Electrical conductivity
κ	Thermal conductivity
κ_e	Electronic thermal conductivity
κ_l	Lattice thermal conductivity
T	Absolute temperature
zT	Dimensionless figure of merit
n	Carrier concentration
e	Electronic charge
μ	Carrier mobility
k_B	Boltzmann constant
E_f	Fermi level
h	Planck's constant
m^*	Effective mass
L	Lorentz number
η	Power generation efficiency
T_H	Temperature of hot junction
T_C	Temperature of cold junction
ε	Carnot efficiency
Q	Heat
Π	Peltier coefficient

Nomenclature

t	Thickness
w	width
$S^2\sigma$	Power factor
V_H	Hall voltage
I	Current
B	Magnetic field
E_a	Activation energy
E_b	Binding energy
α	Incident angle
ϕ	Azimuthal angle
β	Tilt angle
C_v	Specific heat at constant volume
v	Velocity
l	Mean free path
σ_s	Stress
ε_s	Strain
Δl	Change in length
L	Length
E	Modulus of elasticity
K	Bulk modulus
G	Modulus of rigidity
ν	Poisson's ratio
E'	Storage modulus
E''	Loss modulus
S	Stiffness
$\text{Tan}\delta$	Damping factor

Abbreviations

Ag NRs	Ag nanorods
Ar	Argon
BSE	Back scattered electron
CB	Conduction band
COP	Coefficient of performance
CVD	Chemical vapour deposition
DC	Direct current
DFPT	Density functional perturbation theory
DFT	Density functional theory
DOS	Density of states
EDX	Energy dispersive X-ray
FESEM	Field emission scanning electron microscope
FWHM	Full-width at half maxima
GLAD	Glancing angle deposition
HRTEM	High-resolution electron microscope
IPA	Isopropyl alcohol
JCPDS	Joint committee on powder diffraction standards
LA	Longitudinal acoustic
MFC	Mass flow controller
nm	Nanometer
NPs	Nanoparticles
NRs	Nanorods
1D	one-dimension
PGEC	Phonon glass electron crystal
PLEC	Phonon liquid electron crystal

Nomenclature

PPMS	Physical property measurement system
PVD	Physical vapour deposition
RF	Radio frequency
SAED	Selected area electron diffraction
S-NI	Sinus nanoindentation
TA	Transverse acoustic
TE	Thermoelectric
TEDs	Thermoelectric devices
TEM	Transmission electron microscope
TF	Thin film
UNHT	Ultra-nano hardness tester
UTM	Universal testing machine
VASP	Vienna Ab initio Simulation Package
VB	Valence band
XPS	X-ray photoelectron spectroscopy
XRD	X-Ray diffraction