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| Title        | A numerical investigation and optimization by machine learning for the growth of InGaSb crystals with a flatter interface by Vertical Gradient Freezing method under microgravity and normal gravity conditions |
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## Abstract of Thesis

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| Name ( Rachid Ghritle )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                   |
| Title                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | A numerical investigation and optimization by machine learning for the growth of InGaSb crystals with a flatter interface by Vertical Gradient Freezing method under microgravity and normal gravity conditions<br>(微小重力下および地上での垂直勾配凝固法を用いた平坦界面を有するInGaSb結晶成長に関する数値解析と機械学習による最適化) |
| <p><b>Abstract of Thesis</b></p> <p>Semiconductor materials form the fundamental basis of modern electronic devices. Among them, InGaSb, an III-V compound semiconductor, has gained significant interest due to its tunable properties, such as lattice constant and wavelength. This unique characteristic makes InGaSb suitable for various applications, including thermophotovoltaic devices, gas sensors, and infrared detectors. High quality crystals are naturally desirable as substrates for device applications. However, the growth of such homogeneous InGaSb alloy bulk crystals on Earth is difficult because of the adverse effects of natural convection, compositional segregation, etc. These undesirable effects can be minimized under microgravity, an appropriate environment for investigating the growth kinetics and gaining deeper insight into the transport phenomena. Additionally, employing appropriate growth conditions is vital to prevent undesirable solid-liquid interface deformations and ensure compositional uniformity. In this regard, we conducted a comprehensive numerical analysis to determine the optimal conditions for achieving an ideal flat interface shape during InGaSb crystals growth using a combination of different techniques.</p> <p>In the first place, as it is important to employ accurate physical properties in our numerical model, the diffusion coefficient of GaSb in InSb melt was estimated by using the microgravity experimental results performed onboard the International Space Station, where the effect of natural convection was minimized. Furthermore, it was deduced that the growth rate is dominated by the solute diffusion in the melt. the crystal growth rate was well explained by adopting a diffusion coefficient with function of GaSb concentration, obtained by analyzing the available experimental results and utilizing Bayesian optimization.</p> <p>Then, the growth of high-quality InGaSb crystals by Vertical Gradient Freezing (VGF) method under microgravity was numerically simulated, with a focus on controlling the growth interface which directly affects the quality and homogeneity of the grown crystals. Initially, Bayesian optimization was utilized to search for the most favorable temperature gradient that promotes a desirable flatter growth interface shape. Afterwards, an adaptive control recipe (reinforcement learning model) was developed. The system was subjected to a lower temperature gradient near the feed crystal and to crucible rotation with a rate ranging according to the obtained optimal strategy. As a result, the interface deformation is considerably reduced, and a flatter growth interface could be maintained. The growth rate and solute concentration uniformity were also improved.</p> <p>Subsequently, the growth of InGaSb crystals by VGF method under normal gravity was numerically investigated. In order to obtain a flatter growth interface and better compositional uniformity in the melt, the applications of crucible rotation and external magnetic field are considered. We used Bayesian optimization to optimize the related control parameters. Such an optimization has led to a significant reduction in the growth interface deflection and a flatter growth interface was maintained during the entire growth process. Strength of natural convection in the melt was minimized and melt solute uniformity was improved. The growth rate was also increased without compromising crystal quality.</p> <p>The findings of this research study demonstrate the effectiveness of employing crucible rotation, external forces, and optimized temperature gradient for controlling the growth interface shape and composition uniformity. Additionally, machine learning proves to be a valuable tool for the fast search for optimal growth parameters. This thesis not only contributes to a deeper understanding of InGaSb crystal growth process but also can serve as a foundation for future ground experiments.</p> |                                                                                                                                                                                                                                                                                   |

論文審査の結果の要旨及び担当者

| 氏 名 ( Rachid Ghritli )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |     |     |                      |
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| <p>論文審査の結果の要旨</p> <p>半導体材料は現代の電子デバイスの基本的な基盤であり、中でもIII-V 族化合物半導体である InGaSb は格子定数や波長などの調整可能な特性により大きな関心を集めている。この特性により、InGaSb は熱光起電力デバイス、ガスセンサー、赤外線検出器などのさまざまな用途に適している。高品質の結晶はデバイス用途の基板として当然望ましいものの、均質で高品質なInGaSbバルク結晶を地上で成長させることは、自然対流や組成偏析などの悪影響により困難である。これら影響は、微小重力下では最小限に抑えることができる。さらに、固液界面の変形を防ぎ、組成の均一性を確保するには、適切な成長条件を探索することが不可欠である。そこで本論文では、さまざまな手法を組み合わせ、InGaSb結晶成長中に理想的な平坦な界面形状を達成するための最適条件を決定するために、包括的な数値解析を実施した。</p> <p>まず、数値モデルでは正確な物性値を用いることが重要であるため、自然対流の影響を最小限に抑えた国際宇宙ステーションでの微小重力実験結果を用いて、InSb融液中のGaSbの拡散係数を推定した。さらに、成長速度は溶融物中の溶質の拡散によって支配されていたことが特定できた。宇宙実験で得られた結晶成長速度は、ベイズ最適によって得られたGaSb 濃度の関数を伴う拡散係数を用いることにより良好に説明された。</p> <p>次に、成長結晶の品質と均一性に直接影響を与える成長界面の制御に焦点を当て、微小重力下での垂直勾配凍結(VGF)法による高品質InGaSb結晶の成長について数値解析を行った。最初にベイズ最適を利用してより平坦な成長界面形状を促進する最も好ましい温度勾配を探索した。その後、適応制御レシピ(強化学習モデル)を開発した。システムは供給結晶の近くでより低い温度勾配にさらされ、得られた最適戦略に応じた範囲の速度でるつぼ回転を付加した。その結果、界面の変形が大幅に軽減され、より平坦な成長界面を維持することができ、成長速度と溶質濃度の均一性も改善された。</p> <p>続いて、通常重力下でのVGF 法によるInGaSb 結晶の成長を数値的に調査した。より平坦な成長界面と融液中のより良い組成均一性を得るために、るつぼの回転と外部磁場の適用を考慮した。ベイズ最適を使用して、関連する制御パラメータを最適化した。この最適化により成長界面の変形が大幅に減少し、成長プロセス全体を通じてより平坦な成長界面が維持された。融液内の自然対流が最小限に抑えられ、融液の均一性が向上した。その結果 結晶の品質を損なうことなく成長速度も向上した。</p> <p>本研究結果は、成長界面の形状と組成の均一性を制御するために、るつぼの回転、外力、および最適化された温度勾配を使用することの有効性を実証した。さらに、機械学習は、最適な成長パラメータを迅速に検索するための貴重なツールであることが証明された。 この論文は、InGaSb 結晶成長プロセスのより深い理解に貢献するだけでなく、将来の地上実験の基礎としても役立つ。以上のことより、本研究及び本論文は博士(工学)の学位論文として価値のあるものと認める。</p> |     |     |                      |