The formation mechanism and kinetics of Ni_3GaAs nano-thin films on GaAs

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III-V semiconductors, particularly GaAs, are of great interest due to their exceptional electronic and optical properties. Recent advances in the development of CMOS-compatible contacts for GaAs have paved the way for its integration with silicon-based technologies [1]. Metals such as nickel, platinum, and palladium are being extensively studied for their ability to form ohmic contacts through reactions with GaAs while satisfying the CMOS processing requirements [2]. Among these materials, nickel-based compounds have emerged as a particularly attractive contact material due to their excellent adhesion, low contact resistance, and ability to form uniform metallizations [2]. The use of new materials for nanoscale applications requires precise control of interfacial phenomena such as diffusion, reaction, and phase formation. As device dimensions decrease, it becomes imperative to understand and control the physical properties and stability of interfaces at the nanometer scale.

A thorough investigation of metal–semiconductor contacts is therefore essential for advancing the design and fabrication of scaled devices based on III-V compound semiconductors. The solid-state reaction between nickel thin films and GaAs substrates has been extensively studied. The first phase to form is the hexagonal Ni_3GaAs phase [3]. The growth of the Ni_3GaAs phase is diffusion-controlled and nickel is the predominant diffusing species whereas gallium and arsenic remain essentially immobile [3]. However, the mechanism of atomic diffusion in this phase still remains to be clarified.

In this study, the growth mechanisms of the Ni_3GaAs phase are studied for two samples with Ni films of 20 nm and 100 nm of Ni deposited on GaAs. The initial stages of growth and the kinetics of the Ni_3GaAs phase have been studied using in situ X-ray diffraction (XRD) measurements, transmission electron microscopy (TEM), and atom probe tomography (APT) analysis (Fig. 1a). Two interface configurations were examined: one with a coherent Ni/GaAs interface and the other with an incoherent interface. We validate the hypothesis that variations in XRD integrated intensity are proportional to the thickness of the formed phase by performing direct measurements using TEM and in situ XRD (Fig. 1b). In situ XRD measurements were then carried out during isothermal annealing at different temperatures on two samples with Ni film thicknesses of 20 nm and 100 nm, in order to monitor the growth kinetics of the sole Ni_3GaAs phase formed.

By comparing these findings with nucleation and growth models, we conclude that the growth of the Ni_3GaAs phase at the Ni/GaAs interface is predominantly diffusion-controlled at low temperatures and larger thicknesses (Fig. 1c), whereas it is mainly governed by interface reactions at higher temperatures and smaller thicknesses. The results indicate that the Ni vacancy diffusion mechanism is dominant in this phase, and that there is strong agreement between the Ni_3GaAs growth kinetics observed in nano thin films and those reported for bulk diffusion couples. A possible diffusion mechanism is proposed.

References

[1] Y. Wang, W. K. Loke, Y. Gao, K. H. Lee, K. E. Kian Lee, C. L. Gan, C. S. Tan, E. A. Fitzgerald, and S. F. Yoon, CMOS-Compatible Ti/TiN/Al Refractory Ohmic Contact for GaAs Heterojunction Bipolar Transistors Grown on Ge/Si Substrate, IEEE Trans. Electron Devices **68**, 6065 (2021).

[2] T. Sands, V. G. Keramidas, A. J. Yu, K.-M. Yu, R. Gronsky, and J. Washburn, Ni, Pd, and Pt on GaAs: A comparative study of interfacial structures, compositions, and reacted film morphologies, J. Mater. Res. **2**, 262 (1987).

[3] C.-H. Jan, D. Swenson, X.-Y. Zheng, J.-C. Lin, and Y. A. Chang, On the determination of diffusion coefficients in multi-phase ternary couples, Acta Metallurgica et Materialia **39**, 303 (1991).

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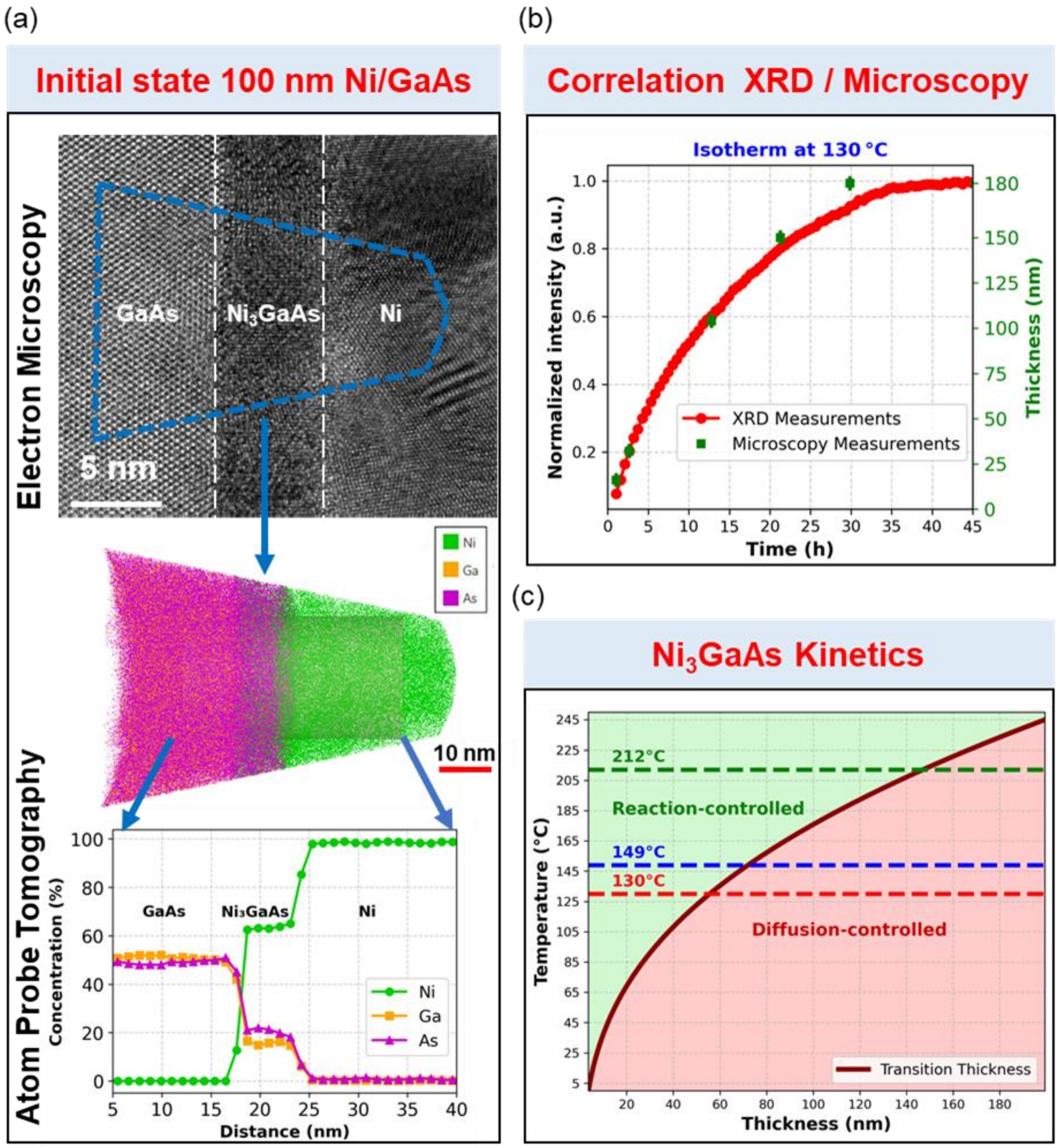

Fig. 1. (a) HRTEM and APT characterization of the samples in their as-deposited state for 100 nm Ni/GaAs sample showing a crystalline interfacial layer (b) Variation of the normalized integrated intensity (red curve with circle)) of the Ni_3GaAs XRD peak as a function of time during isothermal annealing at 130°C, along with the thickness variation measured directly by TEM (green squares) using an in-situ XRD measurement stopped after different annealing times at 130°C. (c) Variation of the "transition temperature" between linear and parabolic regime with thickness. The variation of the thickness of Ni_3GaAs formed during isothermal (130,149 and 212°C) is represented with dash lines.