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# Compensating defects in Si-doped AlN bulk crystals

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**Abstract**

The rather low n-type conductivity observed in Si-doped sublimation-grown AlN bulk crystals is explained by the formation of high concentrations of compensating defects. The model is based on the experimental verification of a shallow impurity band formed by Si donors and the presence of acceptor-like electron traps within 1 eV below the conduction band edge. Further it is suggested that the majority of the Si donors is compensated by deep acceptors in the lower half of the band gap. This compensation model is an alternative to the controversially discussed assumption of Si DX center formation.


*Keywords:* AlN bulk crystals; Si doping; Compensation

## 1. Introduction

Effective n- and p-type doping of the extremely wide-band-gap (~6 eV) semiconductor AlN is a prerequisite for its utilization in III-nitride-based optoelectronic devices for the ultraviolet wavelength region [1]. Theoretical investigations predict that doping of AlN is strongly limited by compensating defects such as vacancies and hardly avoidable impurities [2,3]. In particular, n-type doping is expected to be accompanied by an enhanced formation of negatively charged Al vacancies. The impurity O is believed to form DX centers counteracting the electrical activity of other donors. There is still a controversial discussion of theoretical as well as experimental data whether the donor dopant Si forms a DX center in AlN or acts as an effective-mass donor [2–7]. The broad scatter of the Si donor activation energy between 80 and 320 meV is also awaiting a convincing explanation.

Si-doped AlN bulk crystals grown at our institute showed weak n-type conductivity at room temperature [8]. We report here on the compensation mechanism in these crystals.

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## 2. Experimental details

AlN crystals were grown by physical vapor-phase transport in a TaC crucible at temperatures between 2000 and 2200 °C under a 600 mbar nitrogen atmosphere of high purity. Si doping was realized by adding SiC to the AlN source material. The AlN boules showed a columnar structure with strong $\langle 0001 \rangle$ texture and single-crystalline grains of up to 6 mm diameter.

Chemical analysis with respect to the most important impurities was performed by secondary ion mass spectrometry (SIMS). The Si concentrations of $1\text{–}3 \times 10^{20}\,\mathrm{cm}^{-3}$ exceeded those of C and O by at least an order of magnitude.

The electrically active defects were studied by capacitance–voltage (*C*–*V*), admittance, thermoluminescence (TL), temperature-dependent photoconductivity, and electron paramagnetic resonance (EPR) measurements. For the *C*–*V* and admittance measurements Ni Schottky contacts were deposited in vacuum either on the as grown surface or on polished, KOH etched surfaces. Large-area ohmic back side contacts were prepared by silver glue. The temperature-dependent investigation of the Schottky diodes was accomplished by means of a frequency-variable LCR meter and a temperature-stabilized sample chamber (100–700 K). TL curves were recorded in a scanning electron microscope equipped with a cathodoluminescence system enabling a spatial resolution on the μm scale and temperature sweeps from 10 to 450 K. Single-shot electron-beam excitation was applied at 10 K using typical beam parameters of 20 kV and 200 nA. During linear heating to 450 K with a rate of 0.15 K/s the polychromatic luminescence signal was detected by a photomultiplier tube. The TL analysis took retrapping of charge carriers into account, i.e. second-order kinetics [9]. The EPR data were taken by an X-band spectrometer equipped with a helium-gas-flow cryostat.

## 3. Results and discussion

The $C$–$V$ characteristics undoubtedly proved the n-type conductivity of the Si-doped AlN crystals. A typical example of a $C$–$V$ measurement is shown in Fig. 1. The net donor concentrations determined by using the well-known formulas for the depletion layer capacitance [10] amounted to mid $10^{17}\,cm^{-3}$. The SIMS data yielded Si concentrations of few $10^{20}\,cm^{-3}$ exceeding the C and O concentrations by one order of magnitude. If one assumes a high degree of electrical activation of the incorporated Si, the Si donors must be mainly compensated by a high density of unknown acceptors.

Meaningful $C$–$V$ measurement necessitated the application of a high temperature (500 K) and a low frequency (100 Hz) indicating a high thermal activation energy of the conduction electrons. To determine the activation energy we performed frequency and temperature dependent admittance measurements of the Schottky diodes in the freeze-out region of conduction electrons [11]. This is exemplified in Fig. 2 for a sample in which at least two trap levels can be identified to be responsible for the thermal electron activation. In average, activation energies in the range from 0.5 to 1 eV were determined for all investigated samples. This is much higher than one would expect for the ionization energy of the Si donor.

Further information on the presence of trap levels in our samples we obtained by thermoluminescence measurements. A comparison of the TL spectra of Si-doped (Fig. 3) and -undoped (not presented here) AlN crystals shows that trap levels with lower activation energies than about 1 eV are pronounced only in Si containing samples. In particular, the shallow defect level at around 120 meV, that is not detectable in admittance measurements, is

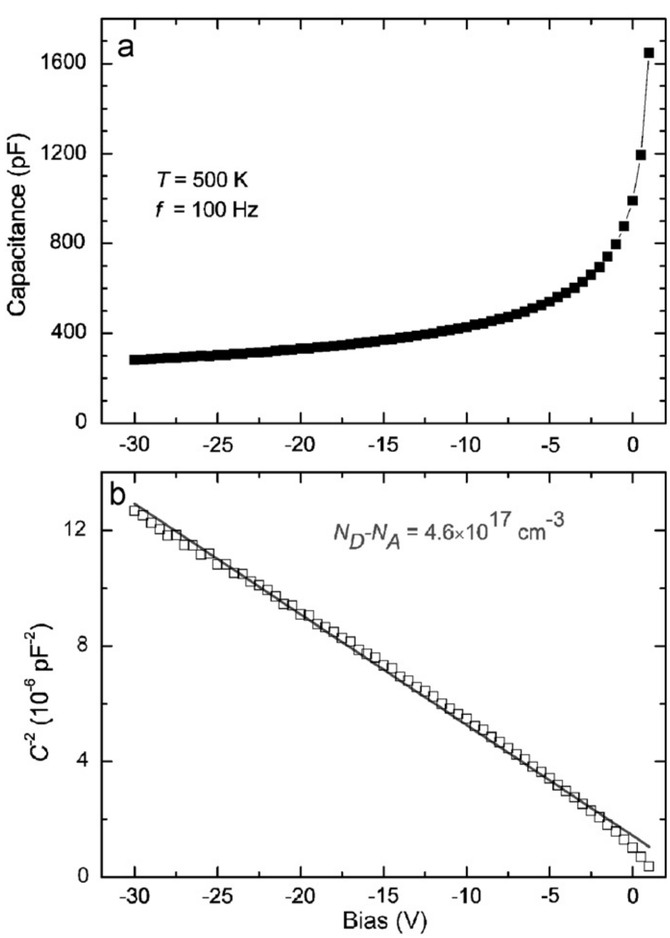


Fig. 1. (a) $C$–$V$ curve of a Ni Schottky contact on the as grown surface of an Si-doped AlN crystal measured at 500 K and 100 Hz. (b) $C^{-2}$ vs. bias plot yielding a net donor concentration of $4.6\times10^{17}\,cm^{-3}$.

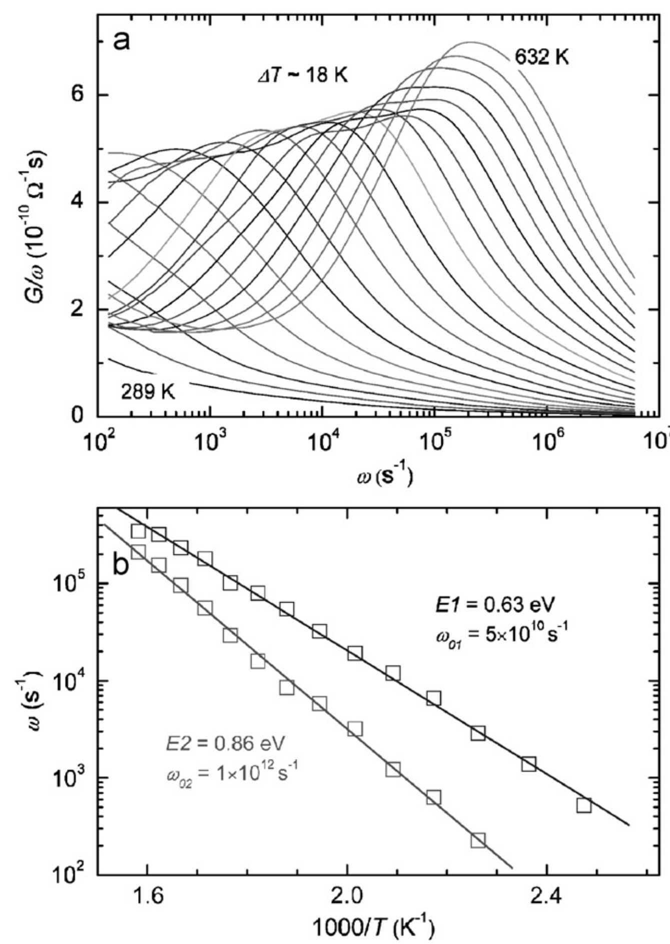


Fig. 2. (a) Frequency and temperature dependence of the conductance divided by the angular frequency (Schottky contact on the as grown surface). (b) Arrhenius plot of the $G/\omega$ peak maxima yielding activation energies of 0.63 and 0.86 eV.