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Microscopic Theory of Gain in a Group-III Nitride Strained Quantum Well Laser

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Abstract

The results of first-principles band structure calculations are incorporated into a many-body laser theory to investigate strain and quantum confinement effects in group-III nitride lasers.

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The study of gain properties in group-III nitride quantum wells is complicated by the incomplete knowledge of band structure properties, and the need for a consistent treatment of strong many-body Coulomb effects. Variations in material quality hamper experiments for investigating band structure properties. As a result, some important material parameters are unknown and much discrepancies exist in others. The strong Coulomb interactions due to high exciton binding energies make it necessary to properly account for the many-body electron-hole effects. The microscopic high-density plasma gain model [1], which is used successfully in infrared III-V lasers [2], may be insufficient because it treats the interband Coulomb interactions as a perturbation, and accounts only for incoherent polarization decay.

This paper describes an approach that involves a first-principles band structure calculation, the results of which are incorporated into a microscopic laser theory. The band structure calculation applies a density-functional method based on *ab initio* pseudopotentials and plane-wave expansions [3]. This method provides a single analytical model for computing the group-III nitride material properties, thus ensuring consistency in the values for the different band structure parameters, and circumventing the discrepancies present in the literature due to different experimental conditions, or different computational methods. Having a complete set of the relevant material parameters allows us to investigate the effects of strain and quantum confinement, in structures such as $InGaN/GaN$ and $InGaN/AlInN$ (Fig. 1).

The quantum well gain is computed by numerically integrating the semiconductor-Bloch equations [1], thereby treating exactly the Hartree-Fock contributions, in particular, that describing the interband Coulomb interactions. Carrier-carrier scattering, resulting in carrier thermalization and polarization dephasing, significantly affects the laser gain. Both effects are treated at the level of the quantum kinetic equations in the Markov limit. This approach circumvents the usual introduction of the phenomenological dephasing time, T_2, whose applicability for wide band gap lasers is still under investigation. Figure 2 shows an example for the calculated dephasing rates.

Our theory predicts that the differences in bandstructure properties, and the significantly stronger Coulomb effects lead to gain properties in nitride-based lasers that are different than those in infrared III-V lasers. The gain peaks are located at lower energies than the exciton resonance, and an absorption resonance remains even at carrier densities that are sufficiently high for gain to occur. Both phenomena are observed in the II-VI lasers (which also have high exciton binding energies), and are indications of strong Coulomb interactions. Specific results involving InGaN/GaN, GaAs/AlGaN and InGaN/AlInN quantum wells will be presented, e.g., the polarization dependence of the laser gain as a function of strain (Fig. 3).

Finally, the detailed treatment of the physical mechanisms contributing to laser gain allows us to develop a gain model, that contains the proper balance between rigor and simplicity, for use in parametric studies of laser configurations. Details of this model and its range of validity will be discussed.

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References

[1] H. Haug and S. W. Koch, *Quantum Theory of the Optical and Electronic Properties of Semiconductors*, 3rd ed. (World Scientific, Singapore, 1994).

[2] W. W. Chow, S. W. Koch and M. Sargent III, *Semiconductor-Laser Physics* (Springer Verlag, Berlin, 1994) Chaps. 5 and 6.

[3] A. F. Wright and J. S. Nelson, Phys. Rev. B 51, 7866, 1995.

Figure Captions

Fig. 1. Computed valence bands near the Γ-point for unstrained GaN (solid curves) and GaN strained to fit on $Al_{0.25}Ga_{0.75}N$ (dashed curves). These results are used to obtain the hole effective masses and the deformation potentials.

Fig. 2. Computed scattering rate for electrons (solid curve) and holes (dashed curve) in a GaN/AlGaN quantum well. The carrier density is $3 \times 10^{12} cm^{-2}$, k is the carrier moment, and a_r is the 2-dimensional exciton Bohr radius.

Fig. 3. TE and TM peak gain versus carrier density for different strain in the quantum well. The laser structure is 6nm $GaN/Al_{1-x}In_xN$ with $x =$(a) 0.13, (b) 0.21 and (c) 0.30.

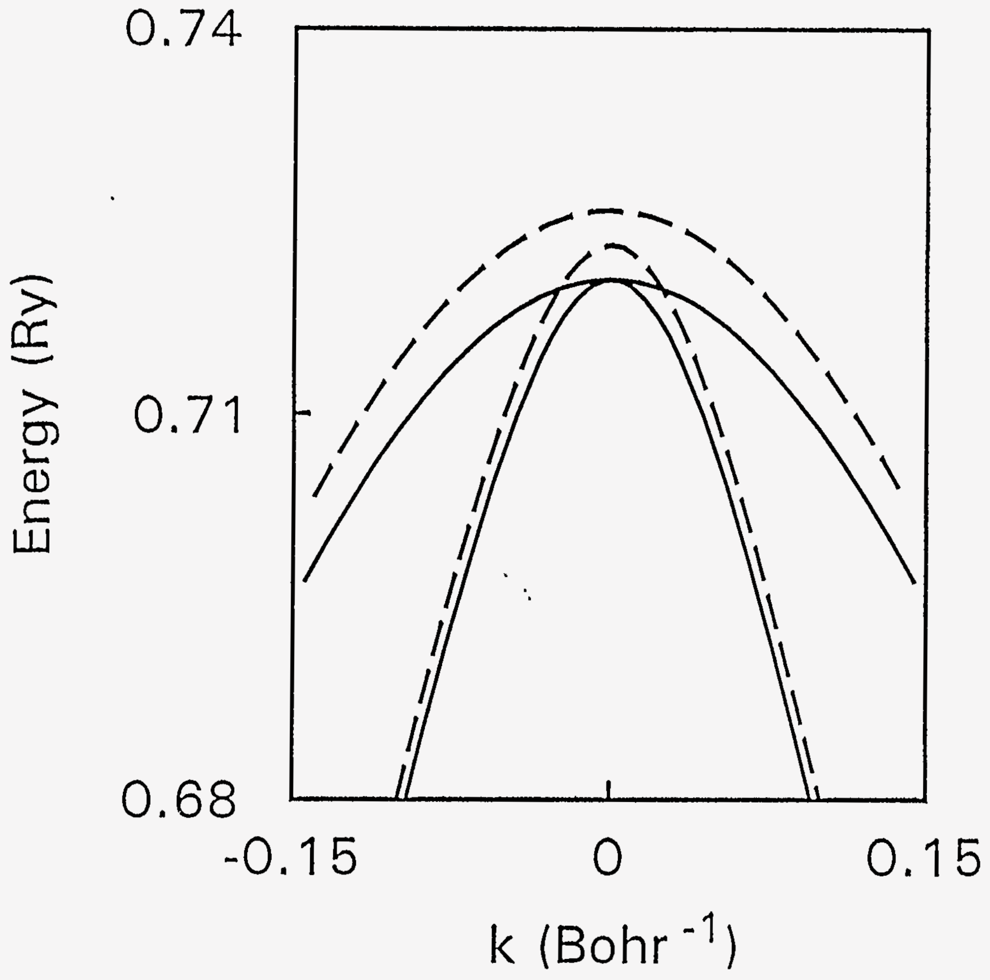

Fig. 1, Chow,...

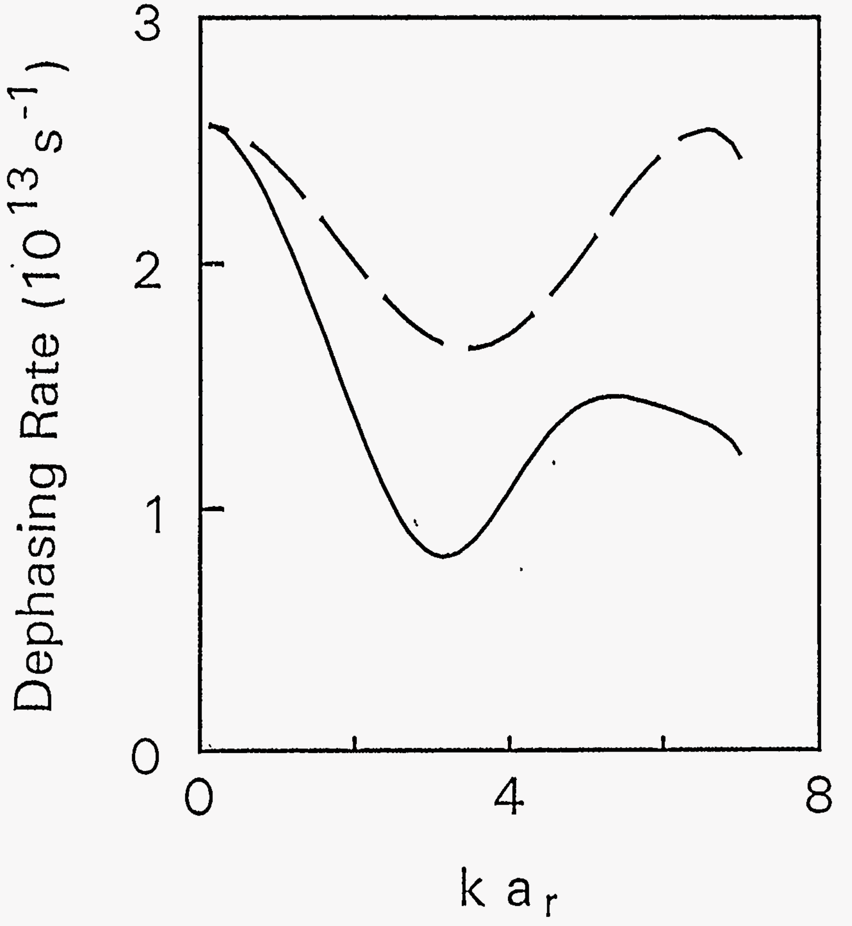

Fig. 2, Chow, ...

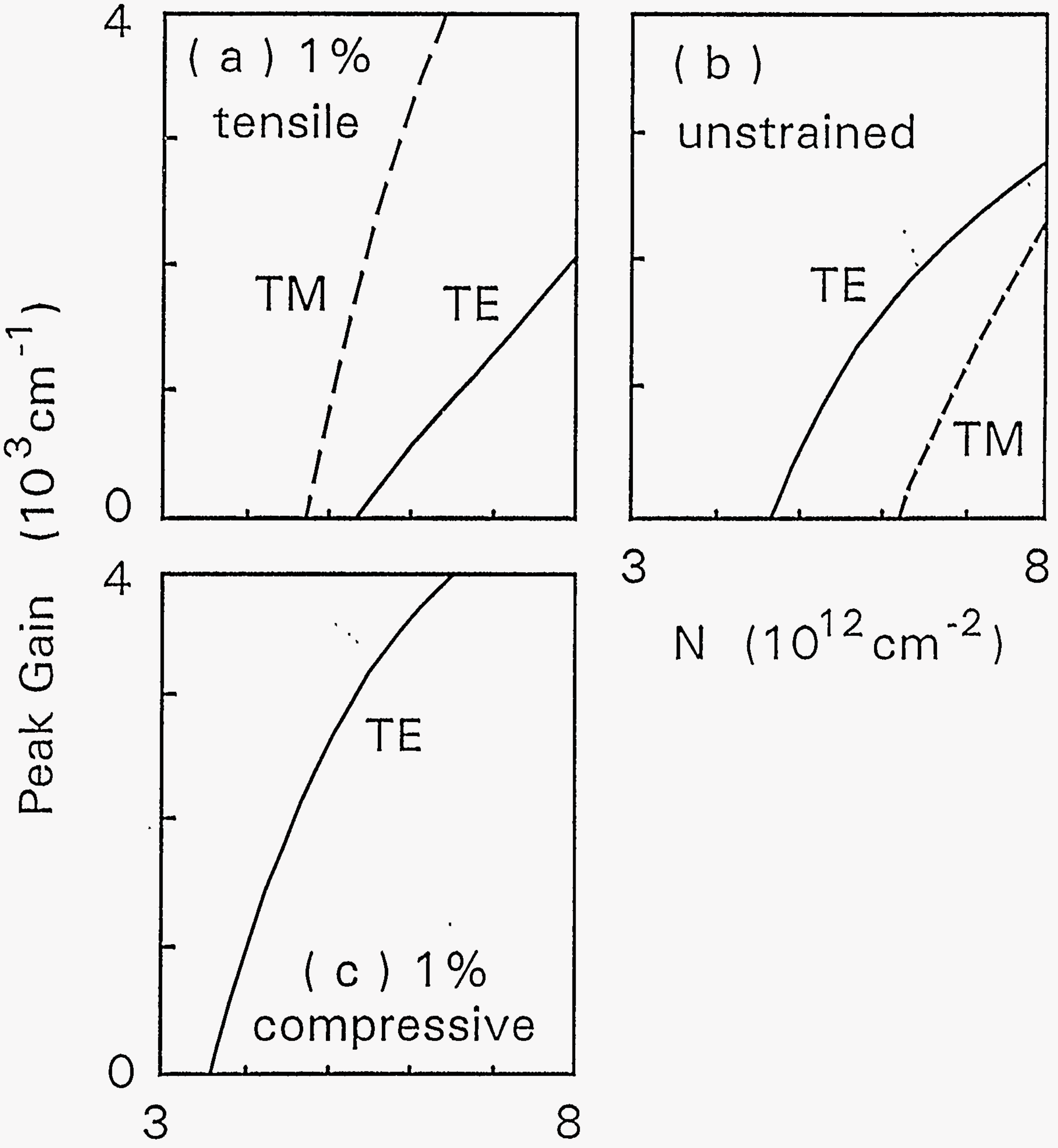
(a) 1%
tensile
TM
TE
(b)
unstrained
TE
TM
(c) 1%
compressive
TE
Peak Gain (10^{3}cm^{-1})
4
0
4
0
3
8
3
8
N (10^{12}cm^{-2})

Fig. 3, Chow,...