



Fourier Analysis and X-Ray Diffraction and Their Applications to the Growth Quality Characterizations In Quantum Cascade Lasers

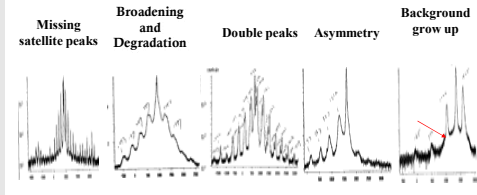
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Motivations:

X-ray diffraction pattern is a Fourier transform of the material layer-structure. By applying the concept of Fourier analysis we hope we can better understand what may have happened during a QCL growth. For Example:



Fourier Transform and X-ray diffraction

$$X(f) = \int_{-\infty}^{\infty} x(t) e^{-i2\pi ft} dt \quad x(t) = \int_{-\infty}^{\infty} X(f) e^{i2\pi ft} df$$

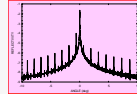
X-ray diffraction pattern is a Fourier transform of the material layer structure. For example, it can be proved that the total scattered wave of x-ray, $G(S)$ can be described as:

$$G(\vec{S}) = \int \rho(\vec{r}) \exp 2\pi i \vec{r} \cdot \vec{S} dV$$

Where $\rho(r)$ is the electron density in the volume element dV . S is the propagation vector bisecting the incident and the diffraction directions.

Methodology:

- A Fourier transform based simulation program is used to simulate superlattice and QCL layers and compare their results with the experimental x-ray diffraction patterns.
- Basic starting structure:
 - 30 periods of lattice matched InGaAs/InAlAs (4.1nm /4.1 nm) superlattice.
 - The simulated result is shown in the right figure
- Next: we setup the layer structure differently and observe how the changes match to the experimental patterns. By adding in the knowledge from Fourier analysis, we try to explain what happened during the crystal growth.

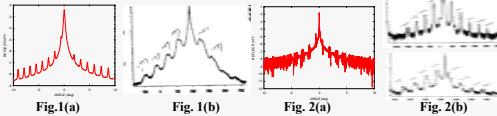


Broadening and Degradation

Two types of broadening effects:

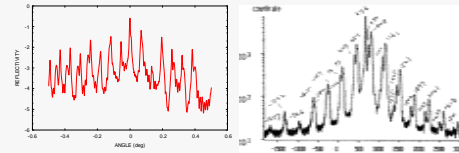
- All satellite peaks broadened – caused by material degradation, mismatch, or a low # of superlattice periods.
- Center satellite peaks stay narrow while satellite peaks further away from the center are wider and lower in amplitude – caused by layer thickness changes.

Simulation Results: 1. Material degradation. 2. Non-strained Chirped Superlattice – layer period thickness gradually changed from 4.5 nm -> 3.7 nm



Double Peaks

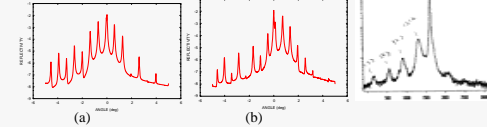
The growth rate changes during the growth. After the QCL layers have been grown for a period of time at a constant growth rate, a sudden change in the growth rate will create a new period. So, basically there are two superlattices— this results in a x-ray diffraction pattern with double peaks. Simulation- strain-balanced QCL: (15/5) periods



Asymmetry

- Results from atomic level lattice mismatch (MOCVD growth chemical concentration changes)
- Tensile strain = shift to the right
- Compressive strain = shift to the left

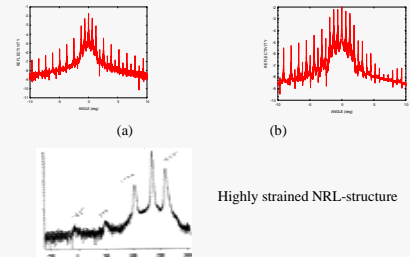
Simulation: (a) InGaAs/InAlAs strain balanced superlattice with (a) In-rich and with (b) Ga rich



Humping Upwards of Background and Loss of Peaks that are Further Away

- When the grown material is highly strained in a strain-balanced material, the satellite peaks go up and the background in the center portion humps upwards as well (see Fig (a) and (b)). If the period cannot repeat very well as discussed in slide-5, there is a loss of periodicity and as a result of the Fourier transform characteristics: only near the center can the satellite peaks be seen. These peaks fade out as they move away from the center.

(a) Strain balanced superlattice In_{0.41}Ga_{0.59}As/In_{0.65}Al_{0.35}As (4.1/4.1) nm
(b) Strain balanced superlattice In_{0.77}Ga_{0.23}As/In_{0.30}Al_{0.70}As (4.1/4.1) nm



Conclusions:

- 1. Fourier analysis helps interpret x-ray diffraction patterns of semiconductor superlattices and QCLs.
- 2. Growth rate changes can be identified from the x-ray diffraction pattern as the decay as well as broadening of outer satellite peaks and multiple peaks on each satellite bin, etc.
- 3. Future works: Relating hetero-Interface quality to the broadening effects of diffraction patterns

