

Review

Fundamentals and engineering of defects

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Abstract

An overview of the important defect types, their origins and interactions during the bulk crystal growth from the melt and selected epitaxial processes is given. The equilibrium and nonequilibrium thermodynamics, kinetics and interaction principles are considered as driving forces of defect generation, incorporation and assembling. Results of modeling and practical in situ control are presented. Strong emphasis is given to semiconductor crystal growth since it is from this class of materials that most has been first learned, the resulting knowledge then having been applied to other classes of material. The treatment starts with melt-structure considerations and zero-dimensional defect types, i.e. native and extrinsic point defects. Their generation and incorporation mechanisms are discussed. Micro- and macro-segregation phenomena – striations and the effect of constitutional supercooling – are added. Dislocations and their patterning are discussed next. The role of high-temperature dislocation dynamics for collective interactions, like cell structuring and bunching, is specified. Additionally, some features of epitaxial dislocation kinetics and engineering are illustrated. Next the grain boundary formation mechanisms, such as dynamic polygonization and interface instabilities, are discussed. The interplay between facets, inhomogeneous dopant incorporations and twinning is shown. Finally, second phase precipitation and inclusion trapping are discussed. The importance of in situ stoichiometry control is underlined. Generally, selected measures of defect engineering are given at the end of each sub-chapter.

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Keywords: melt structure; point defect; segregation; constitutional supercooling; dislocation; dislocation dynamics; thermomechanical stress; grain boundary; facet; twin; precipitates; inclusion

1. Introduction

An overview of the important defect types, their origins and interactions during the bulk crystal growth from the melt and epitaxial processes is given. The attention is focused on semiconductor crystals but the knowledge can be applied to other material classes too.

After defect classification the treatment shows selected thermodynamical and melt-structure considerations. Then zero-dimensional defect types, i.e. native and extrinsic point defects, are introduced. Especially, their

electrical activity and interchange are discussed. The striation genesis and effect of constitutional supercooling are added.

Dislocations and their patterning are discussed next. The role of high-temperature dislocation dynamics for collective interactions, like cell structuring and bunching, is specified. Additionally, the central issues of heteroepitaxy and their control, like arising stresses, bowing, cracking, misfit dislocations and dislocation bending, are specified.

Next the grain boundary formation mechanisms, such as dynamic polygonization, interface instabilities and multinucleation, are depicted. The interplay between facets, inhomogeneous dopant incorporations and twinning is demonstrated.

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Finally, second phase precipitation and inclusion trapping are discussed. The importance of in situ stoichiometry control is underlined.

It is noteworthy that in the past the author presented related lectures at various international schools of crystal growth such as ISSCG-13, ISSCG-15 and IWCGT-3. He also published numerous reviews on crystal defects in journals, conference proceedings and handbooks, see e.g. refs. [1–5]. Thus, in the present chapter only an excerpt of the most important facts is given. For deepening studies the reader may refer to these publications and the literature listed at the end of the paper.

2. Defect classification

Crystal defects, entered in Table 1, are usually classified according to their dimensions.

Zero-dimensional defects are *point defects* comprising intrinsic types like vacancies, interstitials, and, in compounds, antisites as well as unintentionally or intentionally introduced extrinsic atoms as impurities or dopants, respectively.

One-dimensional defects include all kinds of *dislocations*, such as screw and edge dislocations, mixed dislocations, partial dislocations, and dislocation loops. At epitaxial processes one differs between misfit and threading dislocations showing defect lines parallel to the substrate–layer interface and perpendicularly by growing together with the layer surface through the whole epitaxial system, respectively.

Two-dimensional defects are *grain boundaries*, *stacking faults*, *phase boundaries*, *facets*, and *twins*. Low-angle grain boundaries and dislocation cells with tilt angles in the region from arcsec to arcmin, belonging conventionally still to a single crystalline state, are formed by dynamic polygonization and dissipative structuring. In contrast, large-angle grain boundaries with tilt angles of

some degrees are formed by polycrystalline growth. Usually, the indication polycrystal is used above tilt angles of 11–15° when the grain boundary energy loses its dependence on the degree of grain tilt. Facets appear along atomically smooth planes. Their very rapid and discontinuous layer-by-layer growth mechanism incorporates impurities in enhanced concentration and may stochastically create twins by faulty planar nucleus stacking.

Three-dimensional defects include second-phase *particles* (precipitates), intrinsic vacancy conglomerates (microvoids), and foreign particles or bubbles (inclusions). *Precipitates* and *microvoids* are formed by condensation of intrinsic point defects, whereas *inclusions* are melt-solution droplets, gas bubbles, and foreign microparticles incorporated at the growing interface.

Mostly, the kinetics of the defect classes is interlinked. For instance, the conglomeration of vacancies forms spatial microvoids. The climb of dislocations requires the absolute assistance of point defects. Low-angle grain boundaries are formed by dislocation dynamics, etc.

3. Thermodynamic considerations

Principally, defects exhibit heightened energetic potential. In comparison with ideal crystal structure dislocations, grain boundaries and second phase particles show a marked energetic excess. Thus, there is a gain of energy (enthalpy) when such imperfections can be reduced or even prevented. In contrast, in all crystals and thin films a small content of point defects is always situated in thermodynamic equilibrium producing certain disorder, i.e. increasing entropy, that leads proportionally to the reduction of potential of Gibbs $G = H - TS$, with H – enthalpy, T – absolute temperature and S – entropy. For instance, in a crystal with constituents or vacancies the energetic minimum occurs when a certain content n^* is presented as

$$n^* = N \exp(-E_d / kT) \quad (3.1)$$

with N – total number of sites in a crystal lattice, E_d – point defect formation energy and k – Boltzmann constant [4,6] (Fig. 1). Thus, a crystal absolutely free of point defects could never be realized. This is all the more true when considering the marked portion of non-equilibrium point defects frozen in the course of the crystal cooling from growth temperature down to room temperature (Fig. 1).

The general thermodynamic principle of energy minimization is responsible for collective interaction of stored dislocations in as-grown crystals and thin films. The formation of dislocation junctions and walls reduces the

Table 1
Structural crystal defects classified according to their dimensions.

0-dimensional defects <i>Thermodynamic equilibrium</i>	Atomic size (“point”) defects – intrinsic (vacancies, interstitials) – extrinsic (dopants)
1-dimensional defects <i>Thermodynamic non-equilibrium</i>	Dislocations – edge, screw, 60°, 30°, mixed – mobile, sessile, bunched
2-dimensional defects <i>Thermodynamic non-equilibrium</i>	Stacking faults, twins Grain and phase boundaries Facets
3-dimensional defects <i>Thermodynamic non-equilibrium</i>	Precipitates, inclusions Microvoids (vacancy agglomerates) Bubbles, dislocation clusters

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