Methods for liquid–solid interface shape and location discrimination during eddy current sensing of Bridgman growth

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Abstract

Axisymmetric finite element calculations of the multifrequency eddy current sensor response during vertical Bridgman growth have been conducted for GaAs and CdTe. These are representative of materials that are either ideally (the GaAs case) or marginally suited (CdTe) to eddy current sensing during semiconductor growth by a vertical Bridgman process. The simulations reveal two potential strategies for separately discriminating the interface shape and location. One is based upon a comparison of the sensor’s high and low frequency imaginary impedance components. The former characterizes the interface location and the latter its shape. The second approach exploits the existence of an inflection point (or a peak) in the imaginary impedance response of an absolute (or a differential sensor) as an interface passes through it. This latter approach is less affected by test circuit contributions to the sensor’s high frequency response. Both strategies with either sensor type lead to reasonably precise location/shape characterization for GaAs. The differential sensor coupled with the peak position method offers the best precision for less favorable material systems like CdTe. Even for this worst case material, the interface location can be determined to ±1 mm and its curvature estimated with sufficient precision to be of use for characterizing vertical Bridgman growth processes.

1. Introduction

The vertical Bridgman method is a widely used technique for growing single crystal semiconductor materials [1–5]. In this method, a vertical multizone furnace is used to establish an optimized axial temperature gradient through which is translated an ampoule containing the liquid semiconductor. As the lower tip of the ampoule enters the furnace cold zone, single crystal solid is nucleated and a liquid–solid interface propagates upward through the ampoule. Today, the yield and quality of material grown by this technique is maximized by empirically optimizing the temperature gradient and the axial translation rate for each material system. Essentially, this involves repeated experimentation until a satisfactory material can be grown. Once obtained, temperature set points within the furnace, and furnace translation rate schedules are rigidly controlled from run to run.

When applied to the CdTe system, this approach to process optimization/control has failed to result in high yields of acceptable quality single crystal material. The reasons for this are still not fully understood. Recent modelling of the growth process indicates a strong liquid–solid interface curvature sensitivity to the translation rate [6]. This arises from
the very low thermal conductivity of the CdTe system which retards the dissipation of the latent heat released during solidification and promotes non-ideal concave interface shapes. Reports of significant melt undercooling in the high purity CdTe systems, coupled with the possibility of spontaneous solid nucleation and rapid transient growth, raise the possibility that the liquid–solid interface location (its velocity) and its curvature may be uncontrolled by current growth strategies.

This problem has stimulated interest in the use of eddy current methods for sensing the location and shape of liquid–solid interfaces in CdTe [7]. The approach exploits the large change in electrical conductivity that accompanies the melting of this and many other semiconductors [8]. Electromagnetic finite element methods (FEM) have been applied to the design of encircling sensors for locating and characterizing the interface [7,9]. These calculations have revealed that large changes in the sensor’s impedance accompany a change of interface location or shape, and they have identified the best frequency ranges for observing these effects for a variety of semiconductor materials. CdTe has a low electrical conductivity compared to many other semiconductors, and multifrequency measurements in the 100 kHz to 10 MHz range are needed to characterize the interface [7]. Data collected at the high frequency end of this range have been shown to be dependent on the interface’s location but relatively insensitive to its shape. At lower frequencies ( ~ 500 kHz), the sensor’s response depends on both location and shape. Subsequent experiments with an electromagnetically equivalent model system have verified that these predicted trends can be observed experimentally, though at high frequencies (above 3 MHz), test circuit impedances and sensor parasitics cause an unmodelled shift in the sensor’s measured output [10].

These studies indicate that provided the contributions from interface location and shape can be separated, the signals from eddy current sensors appear well suited for monitoring the growth of CdTe. Several monitoring strategies could be pursued. For example, a sensor could be positioned at a fixed location with respect to the ampoule, and the passage of the interface along the ampoule monitored, or the sensor could be continuously repositioned along the ampoule to coincide with the interface, and the sensor’s position then continuously monitored to track interface location (and measure its velocity). In either case, an anomaly-free protocol is needed for separately discriminating the location of the interface within the sensor and determine its curvature.

Here, the finite element method is used to calculate the multifrequency output of eddy current sensors as a liquid–solid interface is propagated upwards through the sensor. This simulation of a stationary sensor’s response during a simulated growth run is repeated for three different interfaces (flat, concave, and convex) and performed for two material systems (GaAs and CdTe). Earlier studies [7] have shown GaAs to be an ideal material system for eddy current sensing because its high conductivity enables the use of low frequencies where test circuit impedance/parasitics are absent during measurements. CdTe appeared to be a more marginal material system and represents a critical test of the eddy current method. The sensor responses from these simulated growth runs reveal two possible strategies for separating the contributions of the interface’s location from its curvature. One uses the frequency dependence of the complex impedance; the second exploits the observation of a frequency dependent inflection point/peak in the imaginary impedance–interface location relationship for the absolute/differential sensor designs [7]. The location of these points is found to provide good discrimination between interface location and curvature even for the more problematic CdTe material system.

2. Analysis methodology

The problem analyzed is shown in Fig. 1. It consists of a cylindrical sample (of diameter, \( D = 76.2 \) mm) contained within an axisymmetric eddy current sensor. The sample has two regions with electrical conductivities of either the solid or liquid semiconductor at its melting point. These conductivity values were the same as those reported in an earlier study [7]. The interface between the two conductivity regions was allowed to be flat, concave, or convex with a convexity parameter \( \theta = z/D \) of \( \pm 0.333 \) and 0 (\( z \) is the maximum difference in axial coordinates of the interface across the sample). The
liquid–solid interface was then introduced at a height $h = -38.1$ mm below the sensor’s midpoint (see Fig. 1 for the definition of $h$) and the two sensors’ responses at 500 kHz again calculated. The interface was systematically advanced in 3.2 mm increments upwards through, and eventually beyond, the sensor and the two 500 KHz responses obtained. Finally, the response due to an entirely solid sample was obtained. This procedure was repeated for ten other excitation frequencies to cover the 10 kHz to 10 MHz range, and for interfaces with convexities of $\pm 0.333$. The electrical conductivities of the test system were then changed to the values of GaAs, and the entire procedure was repeated for 12 frequencies ranging from 200 Hz and 1 MHz. Finally, the sensors’ responses with the samples removed were obtained for all test frequencies used in the calculations. In all, a total of 877 separate FEM calculations were conducted. Using similar procedures to those described in Ref. [7], the absolute and differential sensor impedances normalized by their empty coil values were obtained from these FEM results.

3. Absolute sensor

Fig. 2a shows the normalized imaginary component of the absolute sensor’s impedance for CdTe at a test frequency of 500 kHz as a function of interface location for each interface shape. Results for GaAs at 10 kHz are shown in Fig. 2b. At these two frequencies, both materials exhibit similar behaviors. Initially, when the interface is beyond the range of the sensor’s electromagnetic field (say $h = -80$ mm), the imaginary impedance has a value that depends only upon the liquid’s electrical conductivity and the fill factor of the coil. If the coil’s fill factor is known, the value of the impedance at a fixed frequency moves downwards from its null (i.e. empty coil) value of $0 + j\lambda$ as the conductivity increases. This data could be used to determine the liquid’s electrical conductivity (and to thus infer the factors affecting it) during applications of the sensor to a real growth process. As the interface propagates upwards through the sensor, $h$ goes from negative to positive, the impedance increases, goes through an inflection and asymptotically approaches a constant

![Finite element model geometry.](image)
value corresponding to that of the solid. The impedance in this latter case again depends only upon the test material’s electrical conductivity and the coil’s fill factor. If the latter remains constant (i.e. the test sample and secondary coil diameters do not change), an impedance measurement in this region could be used to infer the solid’s electrical conductivity and gain insight into the factors that control it (e.g. the average temperature in the sensed volume).

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**Fig. 2.** Calculated impedance variation of the absolute sensor with interface position for simulated growth runs of three interface shapes. (a) CdTe (500 kHz), (b) GaAs (10 kHz).

**Fig. 3.** Variation of the imaginary impedance component of the absolute sensor with interface position for a flat interface at four frequencies. (a) CdTe, (b) GaAs.
The results presented in Fig. 2 indicate that when the interface is located far from the sensor’s center (e.g. $h = \pm 40\ mm$ or more), the imaginary impedance is approximately independent of both its location and curvature. However, as the interface approaches the location of the pickup coil, a strong dependence upon both location and curvature is seen. For both material systems, the imaginary impedance associated with a sample containing a convex interface first begins to increase (towards the sensor’s null value of unity on the imaginary axis) as the interface approaches the sensor’s midpoint from below. If the location of the interface (i.e. $h$) were known independently, the imaginary impedance component at these test frequencies ($10\ kHz$ for GaAs and $500\ kHz$ for CdTe) is directly related to the interface’s convexity. For example, if the outside edge of the interface coincides with the pickup coil location ($h = 0.0\ mm$), the imaginary impedance for GaAs would increase from $0.615$ for a concave interface to $0.715$ for a convex one. A smaller, but still significant shift would occur for CdTe. It can also be seen that the point of inflection shifts to the left as the interface’s curvature changes from concave to convex. Therefore, either the value of the impedance or the position of the inflection point are interfacial curvature dependent.

The response to interface location depends upon test frequency for both materials. Fig. 3a shows the imaginary impedance–position relationship for CdTe with a flat interface at test frequencies of $50\ kHz$, $100\ kHz$, $500\ kHz$, and $5\ MHz$. Analogous results for GaAs at $500\ Hz$, $2\ kHz$, $10\ kHz$, and $1\ MHz$ are shown in Fig. 3b. At very low frequencies (below $50\ kHz$ for CdTe and $500\ Hz$ for GaAs), the rate of change of the electromagnetic flux within the test material is sufficiently low that weak eddy current induction occurs, and both samples are almost electromagnetically transparent. In these cases, the decrease in electrical conductivity associated with passage of the liquid–solid interface through the sensor results in a very small change in the nearly null response of the sensor. At high frequency (above $1\ MHz$ for GaAs and $5\ MHz$ for CdTe), the very high rate of change of flux induces intense eddy currents that are concentrated close to the sample surface (due to the skin effect). In this frequency range, the sensor’s response depends strongly on the coil’s fill factor (i.e. the sample diameter) and progressively less on conductivity as the frequency increases. Thus, the sensor’s response is only moderately affected by the location. The largest changes in response are seen at intermediate frequencies where both the eddy current density and the volume within which it exists are both large.

Fig. 4 shows high and intermediate frequency
results for each interface shape. It can be seen that for GaAs, Fig. 4b, a 1 MHz measurement is independent of interface shape but is a unique (though weak) function of location, whereas the intermediate frequency (10 kHz) impedance monotonically increases as either the interface changes from concave to convex, or as its position moves upwards through the sensor. Thus, measurements at the two frequencies shown in Fig. 4b, in combination with the pre-calculated responses for different interface shapes, could be used to separately determine the interface location and shape. The frequencies required to do this for GaAs are below those where test circuit impedance/sensor parasitics are likely to perturb the response [10].

CdTe exhibits a less ideal response, Fig. 4a. Even at 5 MHz (where test circuit impedance/sensor parasitics begin to significantly contribute to experimental measurements), a small residual dependence upon interface shape is observed. This results in greater uncertainty in the interface’s location determination, and since this needs to be known before the interface can be characterized, it results in a reduced ability to characterize the interface’s curvature. This is further compounded by the smaller differences in intermediate frequency (500 kHz) sensor response to each interface shape. Measurements at very high frequency (suitably corrected for test circuit/sensor parasitic shifts) might overcome this difficulty, and the precision of the interfacial curvature could be improved by developing an analysis for a range of test frequencies.

An alternative, potentially simpler approach is to examine the inflection point in the imaginary component’s position dependence. It is clear from Figs. 3 and 4 that this is a function of test frequency and interface shape. To investigate it in more detail, the imaginary impedance–position relationships for each interface shape, frequency, and material were numerically differentiated with respect to interface position and the resulting peak location (and thus the data’s inflection point) determined. This inflection point position is plotted versus test frequency for CdTe in Fig. 5a and for GaAs in Fig. 5b.

Fig. 5 shows that at high frequencies the inflection point position becomes a progressively weaker function of the interface shape. The inflection point for data collected at 1 or 2 MHz during the simulated growth of GaAs corresponds to an interface that is level with the pickup coil location. This result is valid within ±0.5 mm for all three interface shapes. At lower frequencies, the results of Fig. 5b indicate that a large shift in the inflection point occurs as the interface’s curvature changes from convex to con-
cave. For this material system, measurement of the high frequency inflection point (for example, by axially translating the sensor along the ampoule) could be used to position the sensor at the interface’s location, and lower frequency data (say 10 kHz) could then be used in conjunction with Fig. 5b to infer the curvature. If the axial position of the sensor were simultaneously monitored, the strategy would enable separate discrimination of interface location and curvature.

The lower electrical conductivity CdTe system, Fig. 5a, exhibits a similar behavior to GaAs but at significantly higher frequency. For this system, even inflection point data collected at 10 MHz exhibits a ± 1.5 mm position variability due to interfacial curvature. This degree of uncertainty may still be sufficiently precise for some applications (for example, ensuring that solidification occurs at an optimal location in the furnace), but would enable only qualitative insights into the interface’s curvature to be obtained from lower frequency (say 500 kHz) data. Efforts to make measurements at higher frequency to reduce the variation in the inflection point data would have to contend with test circuit contributions to the overall response. These are likely to dominate measurements in the 10–25 MHz range for most experimental setups. Alternatively, extrapolating inflection point data collected in the 1–10 MHz range out to ~ 50 MHz would reduce uncertainty in location and might enable a more precise determination of curvature.

4. Differential sensor

The physical basis of the discrimination approaches proposed above lies in the expulsion of electromagnetic flux by the skin effect. At high frequencies, a uniformly distributed excitation field of the primary coil exists near its center when no sample is present. When a solidification interface resides within the sensor, the skin depths at high frequency are small in both the solid and the liquid, and the electromagnetic field samples only the outer surface of the test material. In this situation, the interface’s location deep within the sample has little or no interaction with the excitation field, and the sensed response depends only upon the fraction of solid and liquid in a thin annular region at the sample’s surface (i.e. it depends only upon the location of the interface within the sensor and not the radial dependence of the location). Unfortunately, the low conductivity (large skin depth) of CdTe requires the use of too high a frequency for this to be easily accomplished.

If this limitation is to be overcome, some way is
needed to increase the rate of decay of the excitation field into the sample. In earlier work, the placement of pickup coils at the ends of the excitation coil was shown to result in a more rapid convergence of the impedance with frequency for the different shaped interfaces [7]. This arose because the "fringe" field at the top and bottom of the sensor decays more rapidly with radial distance in the sample than predicted by a skin effect alone. This additional mechanism of radial field decay can be exploited in the differential sensor approach to better discriminate between interfacial location and curvature.

Fig. 7. Variation of the imaginary impedance component of the differential sensor with interface position for a flat interface at four frequencies. (a) CdTe, (b) GaAs.

Fig. 8. Variation of the imaginary impedance component of the differential sensor with interface position for three interface shapes at two frequencies. (a) CdTe, (b) GaAs.
Fig. 6 shows the variation in the imaginary impedance of a differential sensor when concave, flat, or convex interfaces are propagated through the sensor. The result for CdTe corresponds to an excitation of 500 kHz whilst that for GaAs was obtained at 10 kHz. In both material systems, the passage of the interface through the sensor results in a peak in the impedance. When the interface lies outside the sensor (so that the sensed region is either solid or liquid), a near null response is obtained. As the interface passes close to the sensor’s midpoint, a peak in impedance is observed, and at the two frequencies referred to above, the position of the peak is a significant function of the interface’s curvature. The position within the sensor where the peak is seen also depends upon the test frequency, Fig. 7.

The position dependence of the impedance at high and intermediate frequencies is shown for three interfaces in both CdTe and GaAs in Fig. 8. It can be seen that for both materials the high frequency data is nearly independent of interface curvature when the interface is located near the center of the sensor. At lower frequency, the position of the impedance peak is a strong function of the interface’s position and curvature.

Fig. 9 shows the position of the impedance peak as a function of frequency for each interface and both materials. The fringe field effect combined with the differential scheme results in a lowering of the frequency at which the peak positions converge for both materials. Thus, using the results shown in Fig. 9, data collected at 500 kHz could be used to locate the interface’s position to better than ±0.5 mm in GaAs. For CdTe, data collected in the 5–10 MHz range would enable the location to be deduced to better than ±1 mm. For both material systems, lower frequency data (say 500 kHz for CdTe and 10 kHz for GaAs) could be used in conjunction with the calculations of Fig. 9 to deduce the interface’s curvature. The precision of the curvature characterization will depend upon the accuracy of the location determination. It is estimated to be on the order of 0.05 of the convexity parameter (i.e. approximately 4 mm for a 76 mm diameter sample) assuming the location is determined to ±1 mm.

5. Conclusions

An electromagnetic finite element method has been used to calculate the response of absolute and differential eddy current sensors during the simulated vertical Bridgman growth of CdTe and GaAs. GaAs was found to be an ideal material system for eddy
current sensing because of its high liquid electrical conductivity and large liquid:solid conductivity ratio. For semiconductor systems of similar (or higher) conductivity, eddy current data collected between 500 kHz and 1 MHz with either the absolute or the differential sensor scheme can be used to locate the position of solidification to better than \( \pm 0.5 \) mm. Less ideal systems such as CdTe require the exploitation of fringe fields at the ends of the excitation coil together with a differential sensing scheme to achieve similar location precision. Once the interface’s location is obtained, lower frequency data can be used to deduce the interface’s curvature with acceptable precision for both material classes.

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