Carrier mobility, band tails and defects in microcrystalline silicon

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Abstract. The development of microcrystalline silicon thin films and devices is briefly reviewed. Transport mechanisms, and the attendant key parameters of carrier mobility, band-tail width and defect density, are linked to film structure and composition. In particular we discuss the wide (but systematic) variations in time-of-flight mobility and its unusual field-dependence. While microcrystalline silicon remains an inferior semiconductor to single-crystal silicon, we propose, and support by means of a computer model, that present device-grade material may be of sufficient quality to justify re-examining whether useful thin-film bipolar devices might be developed. These could find application as more sensitive photo-detectors, and as current drivers in organic LED displays and logic circuits.

1. Introduction

Although hydrogenated microcrystalline silicon (μcSi:H) thin films [1] have been studied for at least as long as their amorphous silicon (aSi:H) counterparts [2], their large-scale exploitation in devices has a somewhat shorter history. Until the mid-1980s it was generally believed that the microcrystalline silicon films with the best electronic properties would contain a high crystalline volume fraction, consistent with the observation that crystalline semiconductors generally possess more desirable electrical properties than amorphous semiconductors – high-mobility transport in delocalised states, and a low defect density. However, at that time, highly-crystalline (> 90%) silicon films were found to contain a high density of electrically-active mid-gap defects [3], some $10^{18}$ cm$^{-3}$ compared with below $10^{16}$ cm$^{-3}$ in as-prepared high-quality aSi:H. Recombination and restricted movement of the Fermi level due to these defects cast doubt over the suitability of microcrystalline silicon for use in solar cells and thin-film transistors, which developed as important technological applications of amorphous silicon [4].

Following more detailed work on the relationships between deposition parameters and film structure in the 1990s, a number of groups developed pin solar cells containing microcrystalline silicon absorber layers [5-7]. Most depositions were made using plasma-enhanced chemical vapour deposition (PECVD), although it was demonstrated that hot-wire (HW) CVD material could perform equally well [8]. The development of single-junction μcSi:H and the ‘micromorph’ μcSi:H/aSi:H tandem solar cells has been reviewed [9].

It is important to distinguish between microcrystalline silicon μcSi:H, which forms the subject of the present work, and other forms of crystalline thin-film silicon such as polycrystalline [10], protocrystalline and polymorphous films [11]. μcSi:H is mixed-phase in nature, with crystalline grains...
20 nm or less in size often aggregated into columns embedded in more disordered material. Significant hydrogen is present, as in amorphous silicon. A key feature is that the cracks and voids present in the highly crystalline films, frequently prepared under high RF powers from a process gas containing around 1% of silane in hydrogen, are diminished or absent in more compact films of good electrical quality, deposited at lower powers and higher silane concentrations. The variation in structure and composition that may be obtained by adjustment of deposition parameters is illustrated schematically in figure 1. Diagnostic tools such as electron spin resonance indicate that defect density reaches a minimum at the transition between growth regimes [12, 13], at a phase composition of roughly equal quantities of microcrystalline and amorphous material. It is commonly believed that this corresponds to the point at which the crystalline column boundaries are suitably passivated, giving rise to optimum performance of both solar cells [6] and thin-film transistors [14].

From an applications point of view, there are a number of important differences between aSi:H and μcSi:H. Most fundamentally, their band gaps are 1.8 eV and 1.1 eV respectively, exerting a strong influence on their optical absorption spectra and on dark current magnitudes. Furthermore, aSi:H behaves as a ‘classical’ disordered semiconductor with a largely exponential Urbach tail reflecting the joint density of states, whereas the absorption spectrum of μcSi:H bears a stronger similarity to that of crystalline silicon, as illustrated in figure 2, and is constrained by momentum-conservation, characteristic of an indirect semiconductor, as well as energetic considerations. The photovoltaic efficiency of a stabilized aSi:H solar cell is similar to its μcSi:H counterpart, taking into account that the former suffers more markedly from light-induced degradation, but the deposition rate of good-quality microcrystalline films is lower. This is exacerbated by the fact that a rather thicker μcSi:H absorber is desirable to compensate for its lower optical absorption coefficient in the visible region of the spectrum. Thus it is currently somewhat more economically favourable to produce amorphous silicon modules, although improvements in deposition rate [15] and light-trapping [16] (to maximise the optical path length and reduce the thickness required) may influence this in future. The so-called ‘micromorph’ tandem solar cell, in which the bottom cell is μcSi:H and the top cell aSi:H, has been developed extensively [9] and is now in commercial production. As well as improving module efficiency over a single junction by 2 to 3% the total absorber layer thickness may be reduced, which reduces total deposition time, and the thinner aSi:H layer combined with the more stable μcSi:H cell improves overall stability.

Silicon thin-film transistors (TFTs) [17] have proven highly successful commercially as switching elements in active-matrix liquid crystal (LC) displays. An important parameter in this application is the off: on channel resistance ratio, which can exceed $10^6$ in the case of amorphous silicon. Microcrystalline silicon TFTs look unlikely to rival the amorphous device in LC display applications unless stability is a major issue. However the μcSi:H TFT has a lower on-resistance, which means that in principle it can drive more current and switch more quickly than its amorphous counterpart, and is

![Figure 1. Schematic representation of a silicon thin film, after Vetterl et al [6].](image-url)
therefore more suited to applications in photoemissive displays such as organic LEDs, and in digital logic. The lower channel resistance is primarily a result of increased carrier mobilities, discussed in more detail later, and particularly so in the case of holes where an improvement of over 100 has enabled p-channel [18] and ambipolar TFTs [19], and CMOS logic gates [20], to be developed.

In the following sections, we consider carrier transport in microcrystalline silicon, building on the models developed previously for disordered materials such as amorphous silicon, and augmenting them where appropriate. In particular, the multiple-trapping model will be applied in the interpretation of photoconductivity data. Central to this model is the idea that carrier transport takes place in extended states, but the free carrier density is strongly influenced by the presence of localized states, in the form of band tails and defects, and by recombination centres. By studying both transient and steady-state photoconductivity it is possible to develop a consistent picture of the microscopic conduction properties, and to map this to film structure and composition. In optimised solar cells, carrier extraction appears to be substantially improved over amorphous silicon, which suggests that bipolar transistor action might be achievable. Although appropriate devices have not yet been prepared, possible designs and test procedures are considered, and a computer simulation of the characteristics of an aSi:H/μcSi:H heterojunction bipolar photo-transistor is presented.

2. Relationship between structure, composition and transport

2.1. Structural and compositional elements

As discussed above, mixed-phase μcSi:H films contain proportions of both crystalline and amorphous materials. Based on evidence from structural studies [21, 22] we consider the topology of the crystalline fraction somewhat crudely, as small cubic grains of side g that may coalesce into crystalline rectangular prism-shaped columns of square base width w and height (in the growth direction) h. This is shown schematically in figure 3(a). We assume the columns are disposed some distance apart, and may be separated by voids, by disordered material, or by a combination of the two. In this model, each grain has six faces, which may be considered internal or external to the column, as shown in figure 3(b). At the small grain boundaries, bonds may be unperturbed (figure 3(c)), as within a perfect crystal, deformed by changes in bond length and/or angle (figure 3(d)), or broken (figure 3(e)), resulting in silicon dangling bonds. Furthermore, the ‘space’ between columns may be a void, or may be occupied by some disordered form of silicon, such as ‘standard’ amorphous silicon or a form intermediate between amorphous and crystalline, as illustrated in figures 4(a), 4(b).

We may now examine whether such a model stands up to quantitative considerations, and what predictions might therefore be made from it. Firstly, the model must explain the large difference in defect density observed between highly-crystalline porous material and optimal mixed-phase material.
Figure 3. Highly simplified representation of microcrystalline silicon grains and columns.

Figure 4. Column boundaries – possible configurations.

If closely-spaced columns separated by thin cracks form the bulk, then for a column volume $w^2h$ there is an associated surface area $4wh$ (ignoring the top and bottom surfaces). If the effective bulk defect density is due entirely to the exposed column surfaces, then it may be expressed as

$$N_B = (4wh)N_S/(w^2h) = 4N_S/w$$  \hspace{1cm} (1)$$

For a bare silicon surface, the total surface state density $N_S$ lies in the range $10^{10} - 10^{12}$ cm$^{-2}$ depending on morphology and chemical treatment [23]. Given a typical column width of order 50 nm [21], the calculation suggests that the effective bulk defect density could approach $10^{18}$ cm$^{-3}$, in keeping with spin density [12, 13] and field-effect [3] measurements. The passivating influence of the material between columns thus appears quite strong, reducing the surface density to around 1% of this figure in optimised $\mu$cSi:H. Whether this is due to termination of what would otherwise be dangling bonds, or an internal field-effect retarding carrier motion directed towards the column boundaries, is not clear.

This model may also be used to assess whether the internal boundaries, between small grains within columns, contribute to the overall defect density, and to speculate on the nature of this boundary. The atomic density of silicon is around $5 \times 10^{22}$ cm$^{-3}$, and since the measured defect density in optimised $\mu$cSi:H can be as low as $5 \times 10^{15}$ cm$^{-3}$ as few as one in ten million atoms may contribute a dangling bond. Taking a cubic grain of side $g = 10$ nm, we find that 16% of the atoms lie at the
surface; evidently very few dangling bonds are concealed within columns. TEM and XRD evidence suggests there is also little disordered material within columns [21] and so the internal grain boundaries cannot be preserved in the same way as the column boundaries. A typical sample contains only 3 to 5% hydrogen which, even if all the hydrogen was effective, would leave some 10% of atoms at internal surfaces un-passivated. It thus appears that the grains must undergo some specific structural accommodation that enables the bond order to be preserved across boundaries. This may occur through ‘twinning’, such that adjacent grains share atoms on common lattice sites [22].

2.2. Transport models
Experiments such as transient [24, 25] and modulated [26] photoconductivity and time-of-flight spectroscopy (TOF) [27-30] may be interpreted in terms of a multiple-trapping model [31], and generally support the view that μcSi:H possesses quite extensive conduction and valence band-tails arising from bond distortions in column material. ESR studies [12, 13] reveal significant spin densities, ascribed to dangling bonds at column boundaries. Possible contributions from the amorphous regions outside columns should not be disregarded, though conductive AFM studies [32] indicate, at least for transport through the film, that in more highly-crystalline films amorphous regions generally support only a small fraction of the total transport current. Kocka et al [33] present a transport model which combines reasoning similar to section 2.1 with a proposed density of states (DOS) and electrostatic barriers between crystalline and amorphous regions.

Values of electron and hole mobility, band-tail slopes and integrated defect densities are composition-dependent, and the nature and energetic position of the defects is still open to question. There is no single definitive ‘microcrystalline silicon’ material, owing to the wide range of possible compositions and structures depending on deposition conditions, and thus it is highly unlikely that a single transport model is appropriate for all films in all cases. For example, in amorphous silicon it is accepted that while transport in extended states mediated by multiple-trapping takes place at higher temperatures, band-tail hopping presides at temperatures below 100-150 K. μcSi:H is evidently structurally inhomogeneous which suggests that transport may be similarly anisotropic [33, 34]. There are regions of ‘conducting’ material (crystalline) embedded in a host of ‘less conducting’ material (amorphous), that have led to interest in percolation models of conduction [35], and the effective medium approach [36]. Both have proved successful in predicting certain aspects of transport such as the conductivity-composition transition and temperature-dependence of Hall effect.

As most of the above aspects of transport have already been addressed at some length in the literature, we confine ourselves here to a discussion of a new topic, the composition-dependence of transport in microcrystalline silicon, measured by TOF.

3. Transport measurements
3.1. Composition-dependence of time-of-flight mobility
The variation of electron and hole TOF mobility at 300 K with crystalline volume fraction as determined using Raman spectroscopy ($I_{CRS}$) is shown in figure 5. In all cases, samples were pin structures, with transparent electrodes on each side. Typical i-layer thickness was 4 μm. Preparation conditions are as described previously [15]. Mobility was measured as $\mu = L / tD$, where $L$ is the i-layer thickness, $F = V / L$ is the electric field for a given voltage bias $V$ and $tD$ is the transit time, measured here by the construction illustrated in figure 6(a).

Samples containing more than 30% crystalline material exhibit electron mobilities of 3-4 cm²/Vs, with a corresponding figure of 1-2 cm²/Vs for holes. In comparison with the values indicated for amorphous silicon, electron mobility is a factor of 2-3 higher, whereas the figure for holes is around 300 times higher. For $I_{CRS}$ in the region of 20% both mobilities fall rapidly, which is broadly in keeping with the conductivity transition threshold predicted by percolation theory. However, the mobility values do not attain typical values for aSi:H, as might be expected from percolation theory if transport became controlled by current flow through the ‘host’ material. The electron mobility falls
below that of aSi:H, whereas the hole mobility remains substantially above that of aSi:H. This situation persists with diminishing $I_{\text{CRS}}$ to the limit of detection by Raman spectroscopy. In our PECVD system under the deposition conditions used, this corresponds typically to a process gas concentration $SC$ of around 6.5% silane in hydrogen. Further increase in $SC$ to 10% results in ‘fully amorphous’ material, with the mobilities indicated.

3.2. Dispersion parameters
Multiple-trapping theory applied to a simple exponential distribution of trap states [31] predicts that at a temperature $T$ the pre-transit current $I(t) \propto t^{-1 - \alpha}$, where $\alpha = T / T_0$ is the dispersion parameter for a given band tail slope $T_0$. Additionally, in the same scenario, $\mu(F) \propto (L / F)^{-1 / \alpha}$. Both relationships yield values for $\alpha$, which should be equal. However this is not the case; in this example the pre-transit slope at $T = 300$ K gives $\alpha = 0.50$, whereas the field-dependence of mobility gives $\alpha = 0.87$. The latter case therefore implies a much steeper band tail. Data are presented over a more extensive temperature range in figure 7. It can be seen that while there is good agreement between both methods for both electron and hole TOF on amorphous silicon, the microcrystalline samples yield band-tail slopes that are consistently steeper when measured through the field-dependence of mobility.

Figure 5. Plots of electron and hole TOF mobility at 300 K vs. Raman crystalline volume fraction. Dotted lines indicate the trends of the data. Dashed lines show electron and hole mobilities for fully amorphous samples. Each value is normalised to a sample length to electric field ratio of $10^{-7}$ cm$^2$/V.

Figure 6. (a) Hole TOF transients for a highly-crystalline sample at 300 K, over a range of bias voltages. Pre-transit slope yields $\alpha = 0.50$. (b) Mobilities calculated from transit times plotted vs $L / F$ ratio (log-log scale). Note only weak field-dependence, yielding $\alpha = 0.87$. 

Variation of dispersion parameter $\alpha$ with temperature, for (a) electron TOF, (b) hole TOF. The highly crystalline material corresponds to $I_{CRS} = 60\%$, the amorphous material to $SC = 10\%$ and the low crystalline material to $I_{CRS} \sim 1\%$. The letters P and M denote measurement of $\alpha$ from pre-transit $I(t)$ slope and from variation in mobility with applied electric field, respectively.

3.3. Discussion

TOF data on more crystalline ($I_{CRS} > 30\%$) films are in general agreement with the predictions of multiple-trapping in a disordered semiconductor, i.e. the transits show dispersive behaviour, consistent with the presence of states extending from the band-edge into the mobility gap, and quite low extended state mobilities, somewhat higher than those in amorphous silicon especially in the case of holes, but much lower than in crystalline silicon. However, the unexpected field-dependence of mobility and the strange effects in low-crystalline material suggest the need for a closer look.

Previous studies [29, 30] have tended to concentrate more on lower temperature measurements where a larger portion of the pre-transit region is available for fitting or analysing data parametric in temperature at a specific electric field. This is understandable given the greater difficulty in accurately recording the shorter pre-transit region (compared with amorphous silicon) due to system bandwidth limitations. Brinza et al [37] however, made a comprehensive study of both temperature- and field-dependence of TOF transients for silicon films prepared using the expanding thermal plasma (ETP) technique. They discovered something rather similar to the above, though more extreme - that certain samples exhibited field-independent electron and hole mobilities over a wide temperature range, despite their typical ‘dispersive’ $I(t)$ signatures. They also noted a somewhat enhanced room temperature hole mobility, around 0.01 cm$^2$/Vs. The field-independence was accounted for in a computer model by adding an additional shallow Gaussian density of states to the exponential band tail. The rationale for this was that the ETP material was found to contain nanocrystalline inclusions, and that the states associated with these are suggested to lie in a narrow range within the amorphous silicon bandgap, positioned according to the band offsets.

This idea is interesting, and seems worth pursuing here. From our studies we can identify three aspects of transport in microcrystalline silicon that differ from amorphous silicon, and thus require independent explanation: (a) Hole mobility commensurate with electron mobility for material with crystallinity greater than 30\%; (b) Relatively low electron mobility for low-crystallinity (or Raman amorphous) material; (c) Relatively high hole mobility for low-crystallinity material. We proceed as follows. Above the percolation threshold, both electron and hole currents circulate in predominantly crystalline channels, which offer enhanced hole mobility through reduced disorder, though transport is still limited by trapping and emission. Possibly the extended-state hole mobility is also increased. This could be the case for optimum phase mixture material. As the crystalline content is reduced below the percolation threshold, transport must take place through the lower-mobility ‘amorphous’ material. There would appear to be two additional factors – (i) that barriers to transport may exist between crystalline and amorphous regions, which control current flow, (ii) that the material may be an
‘effective medium’ in which both crystalline and amorphous densities of states (DOS) co-exist. Taking case (i), it seems reasonable to expect an effective mobility lower than in either sub-phase, due to electrostatic barriers. This could account for the reduced electron mobility, though it is generally believed that the energy offset at the conduction band (CB) is small compared with that at the valence band (VB). This raises the question of why hole transport is not adversely affected — holes appear to be more mobile than in amorphous material. We might imagine case (ii) as a superposition of the amorphous and the microcrystalline DOS. At low concentration, the crystalline element may introduce localised states superimposed on the amorphous band tails, reducing the free carrier density in the amorphous material extended states and hence the TOF mobility. At higher concentration, a new set of extended states, rather like impurity bands in a crystalline semiconductor, may result. Depending on their energetic location and capture properties, it seems possible that both could occur simultaneously, i.e. holes propagate in new extended states, but electrons are impeded by new localised states. It may be possible to simulate both the carrier distribution and the effective mobility for such a system.

4. Bipolar thin-film transistor

4.1. Bipolar versus Field-effect

It is interesting to consider the use of BJTs, or a combination of bipolar and field-effect transistors, in certain applications such as photoemissive displays or digital logic, where improved current drive or switching speed may be desirable. As mentioned above, carrier mobilities obtained from curve-fitting to the transfer function of µcSi:H field-effect TFTs exceed 100 cm²/Vs for electrons and 10 cm²/Vs for holes [38]. While the exact figures depend on fabrication details, and in particular on oxygen content of the films, it is clear that they are far in excess of the equivalent values for aSi:H. TFTs are majority-carrier devices however, and cannot provide a direct indication of the prospects for thin-film bipolar junction transistors (BJTs), which rely on transport properties of both carrier types.

In a BJT, minority carriers are injected by a forward-biased emitter-base junction and normally must diffuse across the neutral base region to be swept out at the reverse-biased base-collector junction. Current amplification, defined as the ratio β between collector and base currents may be achieved provided (i) the current injected from emitter to base significantly exceeds that from base to emitter, and (ii) only a small proportion of the current injected into the base (minority carriers) is lost to recombination [39]. There have been few reports of BJT action in amorphous silicon [40, 41], with only modest values of β (2-3) being achieved. To the author’s knowledge, there have been no reports of BJTs fabricated from optimum-phase mixture µcSi:H. However, the broad area of non-crystalline bipolar TFTs is the subject of a US Patent [42], which may have deterred any recent commercial interest.

Based on the steady-state photocarrier grating method, ambipolar diffusion lengths ranging from 100 to 200 nm are obtained for both aSi:H and µcSi:H [43]. These figures can be taken as an indicator of minority-carrier transport efficiency through the neutral base region. In contrast, much improved carrier extraction properties are observed in device-quality µcSi:H pin solar cell absorber layers than in equivalent aSi:H devices, as shown in figure 8. This is especially true in the case of n-side illumination, where hole collection might be expected to be the rate-limiting step. Improved transport properties of both carrier types in µcSi:H would reduce both recombination loss and space-charge accumulation in the BJT. However it should be recognised that the base must be doped in order to obtain transistor action. In aSi:H, minority carrier lifetimes are diminished by doping due to the simultaneous creation of additional defects, although more optimistically a trend of increasing diffusion length with increasing conductivity is shown in µcSi:H [43]. Further, if µcSi:H (bandgap 1.1 eV) is used as base, with an aSi:H emitter (bandgap 1.7 eV), a heterojunction with much improved injection properties is expected. The successful use of aSi:H as a hetero-emitter in high-frequency crystalline silicon BJTs has already been demonstrated [44].
Figure 8. Photocurrent vs. reverse bias voltage for microcrystalline (main figure) and amorphous silicon (inset) pin solar cells. All cells have an i-layer thickness of 4 µm. The symbols >p and >n refer to illumination by 470 nm light (flux $5.1 \times 10^{13}$ cm$^{-2}$s$^{-1}$) from p and n sides, respectively.

4.2. Computer model
As a first attempt, we have modelled an npn thin-film BJT, consisting of n$^+$ aSi:H emitter and collector regions 30 nm wide, identical to those normally used in solar cell simulations, and a p-type µcSi:H base 500 nm wide. Detailed parameters are given in Table 1. To test the BJT, an input signal in the form of a base current is required. The simulator SC-Simul [45] is designed for two-terminal applications, and provides no independent control of the potential of intermediate layers. Therefore an optical signal, uniformly absorbed throughout the base region was applied, giving a photo-transistor structure. The output characteristics of this photo-BJT are shown in figure 9. The effective base current density due to the optical signal is

$$J_B = eG_B W,$$

where $G_B$ is the generation rate and $W$ the base width, and the collector current density is $J_C$. A current gain $\beta = J_C / J_B$, of around 6 is obtained with a neutral defect density of $10^{15}$ cm$^{-3}$. The variation of $\beta$ with defect density is shown in figure 10.

4.3. Summary
Given the large uncertainty in the input parameters, it may be concluded from this model that design of a silicon thin-film based bipolar device with potentially useful levels of current gain may be possible. However, the maximum tolerable defect density stretches the limits of present materials, and the base width and doping level require careful adjustment to obtain a compromise between suitable current gain whilst avoiding ‘punch-through’ breakdown [38]. By making use of microdoping techniques [46] it may be possible to deposit a graded doping profile in the base, providing a built-in field to assist the transport of minority carriers.

| Table 1. Model parameters used in photo-BJT simulation. |
|------------------------------------------------------|
| $E_G$ (eV) | $\mu_{0e}$ (cm$^2$/Vs) | $\mu_{0h}$ (cm$^2$/Vs) | $N_C$ (cm$^3$) | $N_V$ (cm$^3$) | $kT_C$ (eV)$^2$ | $kT_V$ (eV)$^2$ | $E_D$ (eV) | $N_D$ (cm$^{-3}$) | $U$ (eV) |
| n-type aSi:H | 1.70 | 1.0 | 0.1 | $10^{20}$ | $10^{20}$ | 0.1 | 0.15 | 1.1 | $10^{19}$ | 0.25 |
| p-type µcSi:H | 1.12 | 50 | 20 | $10^{20}$ | $10^{20}$ | 0.02 | 0.034 | 0.56 | varied | 0.2 |

Notes:
Key: $E_G$ energy bandgap; $\mu_{0e}$ free electron mobility; $\mu_{0h}$ free hole mobility; $N_C$ effective density of CB states; $N_V$ effective density of VB states; $kT_C$ CB tail slope; $kT_V$ VB tail slope; $E_D$ defect peak energy; $N_D$ defect density; $U$ correlation energy. All energies measured relative to $E_V = 0$

1 Fermi level positions: n-type aSi:H 1.5 eV, p-type µcSi:H 0.28 eV
2 Electron and hole capture coefficients into CB and VB tail states: $10^{-9}$ cm$^3$s$^{-1}$
3 Electron and hole capture coefficients into (i) neutral defects: $5 \times 10^{-9}$ cm$^3$s$^{-1}$, (ii) charged defects: $5 \times 10^{-8}$ cm$^3$s$^{-1}$
5. Conclusions

Microcrystalline silicon thin films of mixed-phase composition show good optoelectronic properties, which are largely resistant to light-induced degradation. This enables them to be used in single-layer and tandem solar cells of comparatively high stable efficiencies. Improvements in deposition rate have been achieved without seriously compromising material quality, although presently this remains a disadvantage in comparison with amorphous silicon. Field-effect transistors show improved bias stability, current-handling and switching speeds, enabling a wider range of potential applications such as drive elements for organic LED photoemissive displays. The enhanced performance of p-channel devices due to the much higher hole mobility offers the potential to develop CMOS logic applications.

Transport landscapes based around the structure of the device-grade mixed-phase material, as examined using Raman spectroscopy, electron microscopy and x-ray diffraction, have been developed. Optoelectronic properties through the film can be explained semi-quantitatively in terms of transport via columnar structures consisting of crystalline grains, in which the column boundaries are passivated by a combination of disordered material and hydrogen. Remaining unsatisfied bonds give rise to mid-gap defects as in amorphous silicon, and band tails result from bond distortions within the columns.

A multiple-trapping model based on this scenario appears to satisfy most aspects of the measured transport behaviour, at least in the case of transient photoconductivity. In general, the conduction band tail has a similar or slightly steeper slope than in amorphous silicon, around 20 to 25 meV, though the valence band tail is noticeably steeper, at 30-35 meV compared with 45-50 meV. Electron time-of-flight mobility at 300 K for comparable sample geometries is two or three times higher in microcrystalline than amorphous material, approaching 5 cm$^2$/Vs at 300 K. Hole mobility is dramatically larger, by a factor of several hundred, and can reach 1.5 cm$^2$/Vs. In order to fit the multiple-trapping theory a lower attempt-to-escape frequency for holes trapped in the valence band is required. Other measurements such as Hall-effect suggest that transport is sensitive to potential barriers at column boundaries. The Hall mobility represents an average value, and hence is lower than in the above case and is Fermi-level position (doping) dependent. However, the trend towards increasing mobility in comparison to amorphous silicon remains in evidence. Field-effect measurements, particularly on top-gate TFTs, suggest much higher mobility values than are obtained from time-of-flight, due possibly to the higher crystalline content at the tops of the columns. To what extent transport in these materials is anisotropic remains an open question, but there are a number of direct and indirect measurements suggesting this is the case. Given the highly asymmetric structure development, it is possible that the effective medium parameters are quite different along the film, compared with through the film, which may also be anticipated to modify the percolation threshold.
Our understanding of transport in lower crystalline fraction material is incomplete. Based on time-of-flight measurements, hole mobility persists at a greatly enhanced level down to some 30% Raman crystalline volume fraction. Below this, both the hole and the electron mobilities appear to fall, and poor electronic quality material is obtained, in which the electron mobility falls below that of amorphous silicon. However, the spin density and CPM defect shoulder are not significantly greater, suggesting that it is primarily the transport path that is subject to additional disruption. Certain aspects of the transport behaviour are difficult to account for satisfactorily with a simple exponential band-tail model, and lead to inconsistencies in electric-field and temperature dependencies similar to those reported for thin-film silicon prepared by the expanding thermal plasma technique. It could be speculated that in such materials the density of states is influenced by additional compositional effects, which might for example involve sub-bands or the localisation of carriers on small islands of crystalline material, from which there is an additional energy cost for one carrier type (the electron) to escape. This is in contrast to the improved medium-range order proposed as a beneficial element found in the structure of protocrystalline silicon thin films.

Although optimum-phase microcrystalline silicon currently does not deliver a game-changing improvement in optoelectronic properties, it is demonstrably better than amorphous silicon in a number of respects. Improved transport properties, especially in the case of holes, opens up the prospect of designing bipolar devices. Models based around the parameters obtained from transport measurements predict a best-case scenario in which a bipolar thin-film TFT with a useable current gain could be realised. While a detailed study of potential benefits has not yet been carried out, there is the prospect that if such devices could be successfully fabricated they might find use in peripheral current drive applications, similar to BiCMOS crystalline silicon technology, and in thin-film digital logic where current amplification may be beneficial at certain nodes, for example to improve fan-out.

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