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SURFACE SCIENCE APPLIED TO THE DEVELOPMENT OF ECONOMICAL PHOTOVOLTAIC SOLAR CELLS

1) The effect of dopants on chemical vapor deposition - a surface potential model.
2) Surface segregation of impurities.
3) Silicon recrystallization using a thin Al - layer on carbon.
4) Effect of structure and impurities on surface states.

SURFACE STRUCTURE AND ELECTRONIC PROPERTIES OF MATERIALS

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AVS - Chicago 1974

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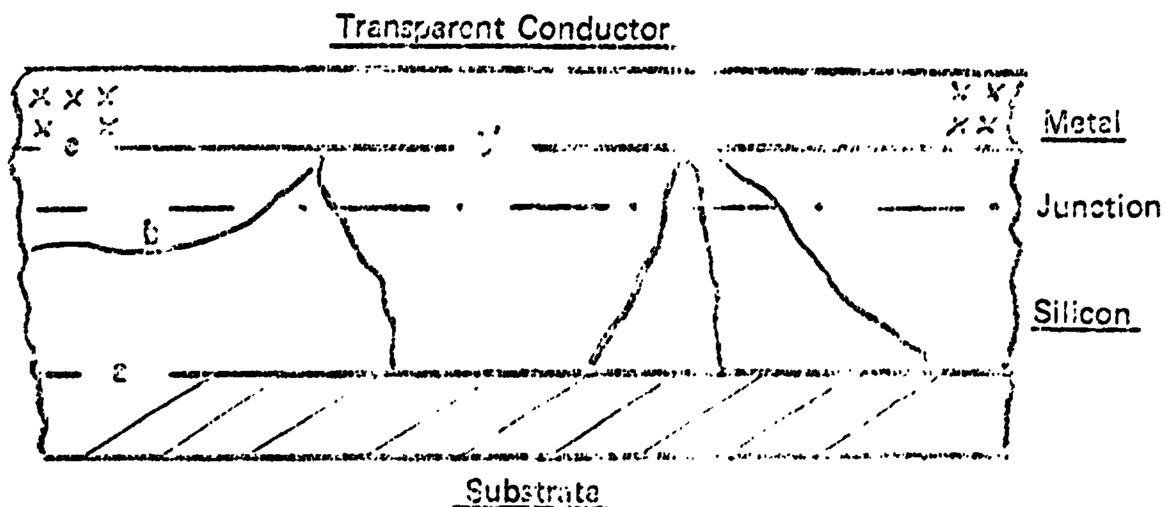
RESEARCH APPLIED TO THE DEVELOPMENT OF THIN FILM POLYCRYSTALLINE SOLAR CELLS

An economically competetive solar cell consists of a substrate on which a 100 μ thick silicon layer is deposited, covered by a transparent conductor containing a metallic grid.
The problems to which research is directed are identified in the cell by the letters a, b, b', c.



Research Areas:

a) Low temperature catalysis of the decomposition of SiH_4, $SiCl_4$ on a low melting point substrate material (e.g. Al) to form large area silicon sheets.
Research tool: molecular beam deposition.

b) Catalysis of large grain crystallization by use of suitable impurities.
Segregation of impurities onto grain boundaries.
Research tool: low energy electron diffraction, Auger spectroscopy.
a,b,b',c. Dependence of electronic surface states on impurities.
Research tool: photoelectron spectroscopy, energy loss spectroscopy.

PROGRAM OBJECTIVE

ANALYZE INFLUENCE AND BEHAVI 'R OF SURFA
AND INTERFACES

DURING CVD FILM DEPOSITION
EFG SHEET FORMATION
CELL LIFE

DETERMINE AND LEARN TO UNDERSTAND, TO CORRECT AND TO USE THE EFFECT OF CHEMICAL COMPOSITION AND PHYSICAL STRUCTURE OF SURFACES AND INTERFACES ON ELECTRONIC STATES.

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The objective of this grant is to employ surface science to the problems associated with the development of economical thin film solar cells: to understand and control the mechanism of chemical vapor deposition, to study substrate - film interaction, to analyze impurity segregation onto surfaces and grain boundaries, to determine the effect of selected impurities on grain growth and to investigate the effect of structure and impurities onto surface states.

We have developed a surface potential model to explain dopant effects on chemical vapor deposition. Auger analysis of the interaction between allotropic forms of carbon and silicon films has shown Si-C formation for all forms but glassy carbon. LEED intensity measurements have been used to determine the mean sqare displacement of surface atoms of silicon single crystals, and electron loss spectroscopy has shown the effect of structure and impurities on surface states located within the band gap. A thin film of Al has been used to enhance film crystallinity at low temperature.

At the present time we perform chemical vapor deposition under externally applied electric fields to test the surface potential model of chemical vapor deposition. We use Auger spectroscopy to identify impurities segregating onto surfaces and interfaces, and we are investigating with electron loss spectroscopy the effect of dopants on surface states.

Future experiments are planned to determine dopant spatial distribution on the surface during chemical vapor deposition, the effect of dopants on chemical vapor deposition reaction kinetics using modulated molecular beam analysis, and the effect of impurities on the activation energy for recrystallization. We plan to use UV electron spectroscopy together with improved energy resolution electron loss spectroscopy to determine absolute energy levels of impurity induced surface states.

WORK PLAN

WORK AREA	PROGRAM	RESULTS
Surface states	LEED intensity data on (111) and (7x7(111) Si	Thesis published. Shows correlation between reconstruction and change in bond strength.
	Electron loss spectra on Si(2x1)(111) Si and amorphous Si.	Report. Shows removal of surface state in midgap by oxygen adsorption.
Impurity segregation	Fracture and analyze large and small grain polycrystal line Si to determine grain boundary impurity segregation.	Report. Difficulties. Si does not reproducibly fracture along grain boundaries. Almost always cleaves. Change experimental procedure.

WORK PLAN

WORKAREA	PROGRAM	RESULTS
Effect of Al on Si crystallinity	Thin layer of Al on C before Si deposition	LB L report. Good crystallinity at low temperature without SiC formation.
Effect of surface charge on deposition	Equipment modification and first measurements.	LBL report, theoretical model submitted for publication.
Analytical work for other groups.	"Get" scanning Auger Analyzing system	"Got" it. Measured boron distribution in ion implanted Si.

GRAIN BOUNDARY SEGREGATION OF BORON IN POLYCRYSTALLINE FILMS.

Experimental results reported in J.Electr.Chem.Soc. (first graph - page suggest, that in chemical vapor deposition together with Boron doping the grain boundary will be completely covered with a monolayer of dopant before doping in the grain can be achieved.

To check this hypothesis, polycrystalline films were deposited onto single crystal substrates covered with a thin nitride layer. Deposition was done by CVD using $SiCl_4$ with B_2H_6 doping by Applied Materials Corporation to a thickness of 200 Å. Estimated concentration of B is $6.6 \times 10^{18}/cm^3$.

The next few graphs show, that polycrystalline silicon, under the conditions investigated up to now almost exclusively fractures by cleavage.

Consequently, Scanning Auger Analysis of fractured surfaces allows up to now no consistent analysis of grain boundary segregation.

/ Efforts continue to find suitable conditions, and an alternate approach to find surface segregation is presented in the next section./

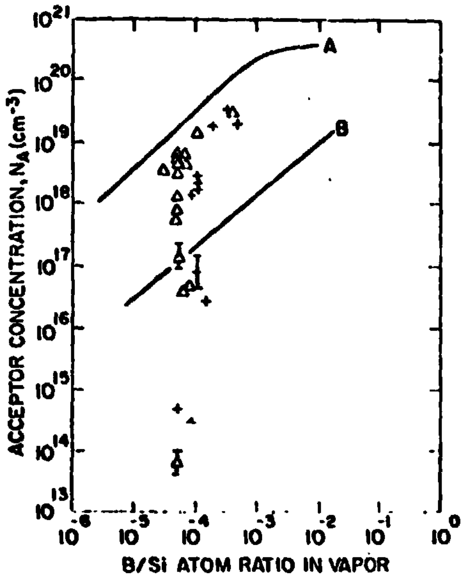

Fig. 2. Acceptor concentration, N_A, vs. B/Si atom ratio in vapor for poly Si samples deposited from SiH_4 at 650°C. △, Thermal SiO_2 substrates; +, fused quartz substrates. Single-crystal doping: -, boron doping of Si from B_2H_6 and $SiCl_4$-H_2 at 1500°K, A (11); B (12).

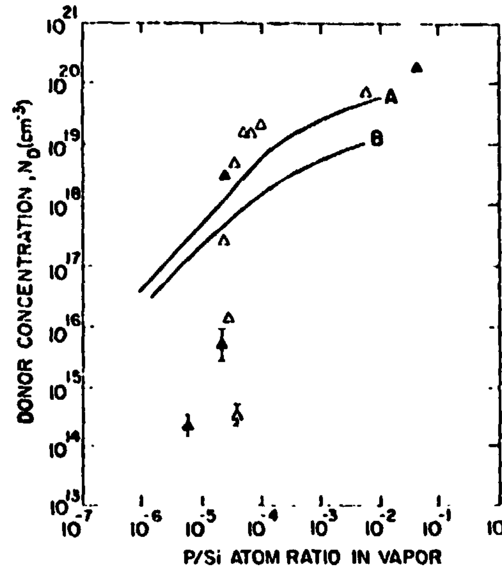

Fig. 3. Donor concentration, N_D, vs. P/Si atom ratio in vapor for poly Si samples deposited on thermal SiO_2 substrates. △ Deposited at 650°C from SiH_4, ▲ deposited at 840°C from $SiBr_4$-H_2. Phosphorous-doped single-crystal silicon, A (14); B (12).

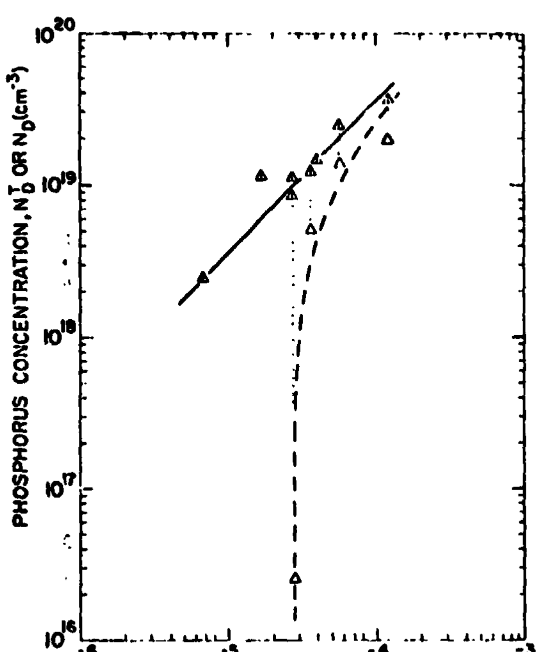

Fig. 4. Total phosphorous concentration, N_D^T, and donor concentration, N_D, vs. P/Si atom ratio in vapor for poly Si deposited from SiH_4 at 650°C. ▲ Total phosphorous concentration, △ donor concentrations, ——— see Eq. [1] in text, - - - - calculated from Eq. [4] in text.

M. E. Cowher and T. O. Sedgwick, J. Electrochem. Soc., SSS&T, Nov. 1972

Typical Grain Boundary Fracture of Fe-12 Mn-0.2 Ti, 1000 X

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S[illegible]face of Pol[illegible] on Si[illegible]onnitri[illegible]e ([illegible]00X)

FRACTURE VIEW OF POLYCRYST. SILICON CLOSE TO SURFACE, (600)

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FRACTURE VIEW OF POLYCR. SI FILM ON SI... [illegible] NITRIDE ([illegible] X)