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STUDIES OF OXYGEN- AND CARBON-RELATED DEFECTS IN HIGH-EFFICIENCY SILICON SOLAR CELLS

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OXYGEN AND CARBON ARE ALMOST ALWAYS PRESENT IN SILICON.

[O] $\lesssim 10^{18}$ / CC , 30 ppma

[C] $\lesssim 5 \times 10^{17}$ / CC , 10 ppma

Oxygen comes from the silicon source or from quartz boats.

Carbon comes from graphite susceptors in pullers.

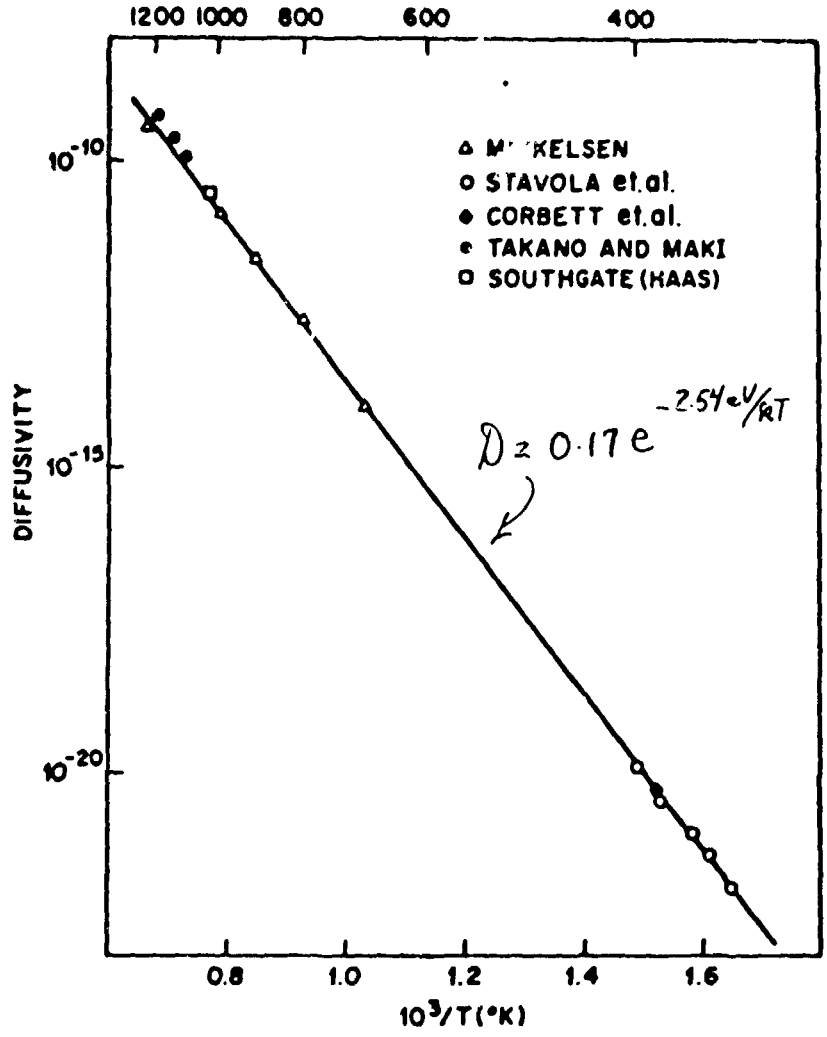
WE KNOW THE CONFIGURATIONS OF THESE IMPURITIES:

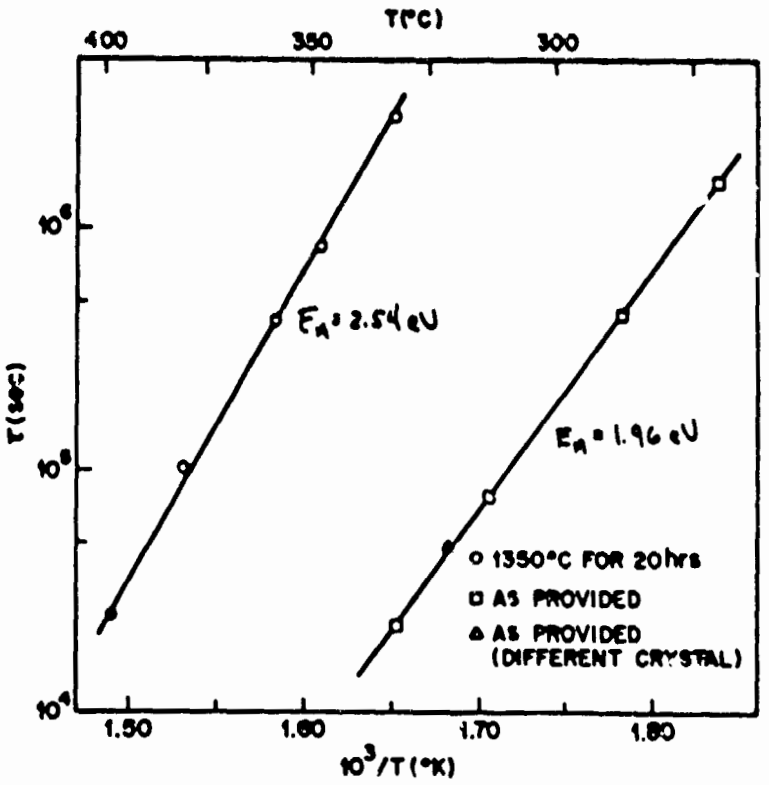
OXYGEN IS A PUCKERED BOND-CENTERED INTERSTITIAL.
(OXYGEN IS QUITE MOBILE.)

CARBON IS A SUBSTITUTIONAL ATOM.
(CARBON IS RELATIVELY IMMOBILE.)

BOTH ARE ELECTRICALLY INACTIVE
IN THIS FORM.

ALTHOUGH THERE HAS BEEN A LOT OF CONTROVERSY AND UNCERTAINTY CONCERNING THE DIFFUSION COEFFICIENT OF INTERSTITIAL OXYGEN, WE NOW KNOW THIS QUANTITY VERY WELL, PRIMARILY BECAUSE OF THE WORK OF STAVOLA AND OF MIKKELSEN.





A MAJOR ADVANCE IS THAT MODERN QUANTUM CHEMICAL CALCULATIONS (SNYDER-ALBANY) CAN TREAT THE DIFFUSION OF OXYGEN QUANTITATIVELY.

BUT STAVOLA ALSO FOUND AN ANOMALOUS DIFFUSION PROCESS IN SAMPLE WHICH HAD A 2 HOUR HEAT-TREATMENT AT 900 C .

THIS ANOMALY REMAINS A MAJOR PROBLEM.

M Stavola et al.

WHY IS THIS DIFFUSION A CONCERN?

MOBILE OXYGEN PRECIPITATES IN A COMPLEX WAY,
AND CARBON MAKES THAT PRECIPITATION EVEN MORE COMPLEX.

CONSIDER A SAMPLE THAT HAS HAD A HIGH TEMPERATURE (E.G., 1300 C) ANNEAL WHICH DISPERSES THE OXYGEN AND CARBON.

FULLER ET AL. (1954 !) FOUND HEAT TREATMENT DONORS BEFORE IT WAS KNOWN THAT OXYGEN WAS IN SILICON.

KAISER, FRISCH AND REISS (1957) OUTLINED THE BROAD PICTURE OF THE PROCESSES:

$$O + O \longrightarrow O_2$$

$$O + O_2 \longrightarrow O_3$$

$$O + O_3 \longrightarrow O_4$$

$$O + O_4 \longrightarrow O_5$$

ETC.

SUBSEQUENT WORKERS USING IR, EPR AND DLTS STUDIES SHOWED THAT THERE IS A HIERARCHY OF DOUBLE DONOR DEFECTS.

SUEZAWA AND SUMINO (1984) SHOWED THAT

TD1 = O_3

TD2 = O_4

TD3 = O_5

TD4 = O_6

TD5 = O_7

TD6 = O_8

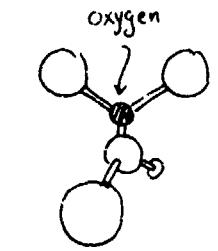
IR STUDIES REVEAL BOTH THE HYDROGENIC AND HELIUM-LIKE STATES OF THESE NINE DOUBLE DONORS.

THE HELIUM-LIKE GROUND STATE IS AT (E - 0.15 eV) FOR THE TD1 AND GETS PROGRESSIVELY SHALLOWER FOR THE REMAINING DEFECTS. THE THEORY OF THIS PROGRESSION HAS BEEN ESTABLISHED (CORBETT, FRISCH, AND SNYDER, 1994).

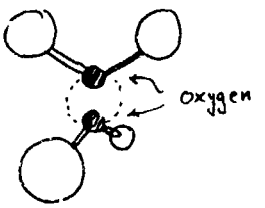
THE DONOR APPEARS TO HAVE A "CORE" WHICH CAUSES THE ELECTRICAL ACTIVITY AND SUCCESSIVE OXYGENS CREATE THE HIERARCHY OF DEFECTS.

"CORE" + n (OXYGENS) + YDn

THERE ARE A NUMBER OF MODELS FOR THE CORE, BUT THE FRONT-RUNNERS ARE THE 'YLID" AND THE (VACANCY+ TWO-OXYGENS), BOTH MODELS ARISING FROM STUDIES AT ALBANY



"Ylid"
or
Split <110> Si-O
Interstitial



$(V \cdot O_2)$

THERE HAS BEEN A GREAT DEAL OF PROGRESS IN THE STUDY OF OXYGEN IN SILICON, AND WE SHOULD SOON UNDERSTAND THIS OLD PROBLEM.

WE ALREADY KNOW ONE OF THE DIFFICULTIES: THE OXYGEN PRECIPITATION PROCESS GENERATES SILICON INTERSTITIALS AND THESE ARE VERY MOBILE AND REACTIVE.

$$(Si)_I + (C)_s \longrightarrow (C)_I$$

$$(Si)_I + (B)_s \longrightarrow (B)_I$$

etc.

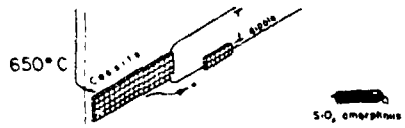
AND THE PRODUCTS OF THE REACTIONS, E.G., THE CARBON-INTERSTITIAL AND THE BORON-INTERSTITIAL ARE VERY MOBILE, REACTIVE AND ELECTRICALLY ACTIVE, AND CREATE OTHER DEFECTS THAT ARE ELECTRICALLY ACTIVE.

FURTHERMORE CARBON SUPPRESSES THE FORMATION OF THERMAL DONORS AT 450° C, BUT APPARENTLY AIDS THE FORMATION OF "NEW DONORS" AT 650° C, AND LITTLE HAS BEEN DONE IN STUDYING THOSE DEFECTS.

RETURN TO THE PRECIPITATION OF OXYGEN.

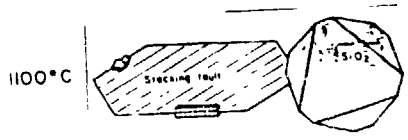
AFTER A 600 °C ANNEAL, THE THERMAL DONORS ARE GONE, AND <110> "RODS" AND "BLACK DOTS" ARE OBSERVED IN THE ELECTRON MICROSCOPE.

BOURRET ET AL. (1983) HAVE SHOWN, USING HIGH RESOLUTION ELECTRON MICROSCOPY, THAT THE RODS ARE COESITE, A HIGH PRESSURE PHASE OF SILICON-DIOXIDE, AND THE DOTS ARE AMORPHOUS SiO_x .



AFTER AN 850° C ANNEAL, THE RODS HAVE DISAPPEARED AND DISLOCATION LOOPS (WITH, PRESUMABLY, COESITE PRECIPITATES) AND LARGER SiO_x DEFECTS ARE OBSERVED IN ELECTRON MICROSCOPY.

AFTER AN 1100° C ANNEAL, LARGE STACKING FAULTS (AGAIN WITH OCCASIONAL DECORATION OF PRECIPITATES) AND LARGE SILICON DIOXIDE PRECIPITATES ARE OBSERVED IN THE ELECTRON MICROSCOPE.



WHY IS ALL THIS PERTINENT TO HIGH EFFICIENCY SILICON SOLAR CELLS?

WE NOW KNOW THAT THERE ARE MANY PROCESS-INDUCED DEFECTS IN SILICON, SOME OF WHICH ARE THE FAST DIFFUSERS, Fe, Ni, Cu, Au, ETC.

ALL OF THESE DEFECTS CAN INTERACT WITH THE OXYGEN- AND CARBON-RELATED DEFCTS. INDEED THE OXYGEN PRECIPITATION IS KNOW TO PROVIDE DEFECTS WHICH ARE HELPFUL IN GETTERING IMPURITIES.

BUT THE NATURE OF THESE REACTIONS IS STILL LARGELY UNKNOWN.