Origins of Nonstoichiometry and Vacancy Ordering in Sc$_{1-x}\square_x$S

G. L. E. H... A. x ...

National Renewable Energy Laboratory, Golden, Colorado 80401

(Received 13 A... 2001; ... 13 D... 2001)

We ... D... ... ($\square$, ...) ... ... Sc$_{1-x}\square_x$ ... x ... B ... ... : (111) ... (112) ... (110) ... . E... ... ... ($\sim 3 \times 10^6$ ...) ...

We ... Sc$_{1-}$ ... ...

FIG. 1. ... $\sim 3 \times 10^6$ ... ($1-\square$) ... LDA- ... 12 ... ($\leq 1/3$).

x- 8,23.

Long range order.

(F . 2) : ( ) : (111). ( ) (111) , (112) .

F x , = 1/6 1 2 1 8 ., ( ) -

3.00

1.00