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Thesis Abstract (Ph.D.)

Modelling, scale-up and design of fluidized bed reactors by Ashok Kumar Vaish Department: Chemical Engineering

1. Introduction

Fluidization is one of the most attractive branches of chemical engineering and during the last three-and-a-half decades, apart from its application in metallurgical ore roasting, limestone calcination, synthetic gasoline and petrochemicals, has spread even to the design of the nuclear reactors. The first large-scale fluidization application in the United States dates to about 1940 and pertains to catalytic cracking of oil vapors. The process was first described by Murphree and coworkers¹. The major breakthrough in industrial scene came in 1942 when the first commercial fluid-bed catalytic plant was put into operation followed by 31 additional plants during the period of the Scoold World War. Fluidization (fig. 1) being an attractive unit operation offers an elegant solution to a wide range of industrial problems. In spite of the continuous investigations on vanous aspects of fluidized bed, design procedures of fluidized bed reactors have not been established.

2. Object of the present investigation

The prime objectives of the present investigation are to (i) characterize the flow regimes under bubbing and slugging conditions (ii) model the gas-solid bubbling and slugging fluidized systems in order to predict the various hydrodynamic characteristics incorporating the scale-up effect, effect of static bed height to bed diameter ratio and impact of particle size (iii) correlate the quality of fluidization with the axial everage pressure fluctuations and axial voidage distribution (iv) further unfold the mysteries of bubbling and slugging phenomena through transient studies (v) propose steady-state and transient models for bubbling and slugging fluidized bed reactors and (vi) propose scale-up and design aspects of fluidized bed reactors.

3. Experimental

A massive experimental set-up, consisting of (i) five laboratory-scale fluidized bed glass columns of 4.5, 7.3, 9.1, 10 and 15 cm in dia (ii) two pilot-scale fluidized bed glass columns of 20.7 and 294 cm in dia and (iii) two multipurpose stanless steel fluidized bed reactors of 10 and 17 cm in dia, was designed and fabricated Extensive experiments were conducted in laboratory scale and pilot scale fluidized bed columns in order to visualise, examine and measure the hydrodynamic characteristics of gas-solid fluidized systems by direct observation, still photos and movie films using about 30 sizes of 13 materials covering a wide range of particle size (0.009 to 0.335 cm) and particle density (1.033 to 7 4605 g/cc).



Fig. 1. Spectrum of gas-solid fluidization,

A Modelling of bubbling fluidized system

Toomey and Johnstone², Davidson and Harrison³ and Partridge and Rowe⁴ suggested that all the gas in excess of what is required just to fluidize the system, passes in the form of bubbles leaving the dense at the minimum fluidization voidage. Kunii and Levenspiel⁵ proposed the characteristics of bubble based on the theories of Davidson and Harrison³. An extensive study regarding the vanous characteristics of bubbling fluidized bed was conducted and models were proposed to (i) predict the extent of bubble-free fluidized bed above minimum fluidizing velocity (ii) estimate the bubble diameter at different heights above the distributor (iii) characterize the flow regimes of bubbling, fluidized systems based on the size of the bubble (iv) predict the onset of free bubbling, vigorous bubbling and turbulent bubbling (v) predict the bed expansion ratio and bed fluctuation ratio, incorporating the scale-up effect and the effect of bed height for three different ranges of particle diameter.

5. Modelling of slugging fluidized system

According to Leva et al^6 , the bubble coalescence occurs rapidly immediately above the distributor in a fluidized bed of coarse particles. The coalescence that leads to the formation of slugs takes place within a height equal to a few bubble diameter / e , within a bed height of the same order as the bed diameter. According to Davidson and Harrison⁷ square-nosed slugs are very common in tubes up to 5 cm diameter and uncommon in large diameter columns. Potter and Thiel⁸ and Carotenute et al⁹ have recently showed that square-nosed slugs occur even in large diameter columns. William and Potter¹⁰ observed experimentally that existing round-nosed slugs broke down into the turbulent regime at a 0.10 m dia bed and 2.5 cm/s in a 0.22 m dia bed. Comprehensive studies were conducted covering various aspects of slugging fluidized bed and models were proposed to (i) predict the minimum bed height required for the onset of round- as well as square-nosed slugging (ii) predict the onset of round- and square-nosed slugging (iii) characterize the flow regimes of round-/square-nosed slugging based on the height of the slug above the distributor (iv) predict the onset of vigorous round-/square-nosed slugging and turbulent round-/square-nosed slugging (v) predict the height above the distributor at which round-/square-nosed slug forms at different flow-rates of fluidizing gas (vi) predict the lengths of round-, square-nosed slugs, lengthy slugs and wall slugs and (vii) predict the bed expansion ratio and bed fluctuation ratio under round-/square-nosed slugging conditions

6. Axial pressure fluctuations and axial voidage distributions

Experiments have been conducted in 10 and 17 cm diameter stainless steel fluidized bed reactors (i) to measure the pressure drop fluctuations at different heights above the distributor at different flow rates of the fluidizing gas, and (ii) to determine axial average voidage distribution in successive zones and average pressure drop per unit length across each successive zone of bubbling/slugging fluidized bed at different flow rates of the fluidizing gas, covering a good range of particle size, bulk density, particle sphericity and density, static bed height to bed diameter ratio and materials of different characteristics. The axial pressure fluctuations and the axial average voidage distributions furnish rough estimate regarding the flow regime of bubbling/ slugging, approximate diameter of the bubbles, approximate idea regarding the type of slugs, type of solid mixing, maximum bed expansion and bed fluctuation. They are of paramount importance in analysing the data from pilot plant tests and in designing the pilot-scale fluidized bed reactors.

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7. Transient analysis

The necessary observations regarding (i) the shape and size of bubbles (ii) the shape and length of different types of slugs (iii) the fluctuations in fluidized bed, top of fluidized bed charge and pressure drop across the fluidized bed were recorded meticulously in 4.5, 7.3, 10, 15, 20.7 and 29.4 cm dia fluidized bed glass columns under different modes of bubbling/slugging at 32 frames per second on movie films. The exhaustive frame-by-frame analysis of movie films regarding the bubbling and slugging phenomenon can be successfully employed in analysing the transient experimental data from pilot-scale and semi-industrial scale fluidized bed reactors

8. Effect of bed height

For a given bed diameter, the bed height controls the flow pattern of fluidizing gas, pattern of solid mixing, mechanism of gas-solid contact, mode of fluidization and the overall efficiency in a gas-solid reactor. Effects of bed height have been exhaustively studied with different materials in (i) minimum fluidizing and bubbling velocities (ii) minimum freely, vigorous and turbulent bubbling velocities, (iii) minimum round-/mixed-/square-nosed slugging velocity (iv) minimum vigorous and turbulent round-/mixed-/square-nosed slugging velocities (v) bed expansion ratio and bed fluctuation ratio under bubbling condition and (vi) bed expansion ratio and bed fluctuation ratio under round- and square-nosed slugging conditions. The bed height plays very significant role in the scale up and design of fluidized bed reactors.

9. Scale-up effect

The bed diameter is one of the dominating parameters in the design of fluidized bed reactors It controls the entire spectrum of the behaviour of fluidized bed under normal and extreme operating conditions. Scale-up effects have been exhaustively stiduled with different materials on various hydrodynamic characteristics of bubbling and slugging fluidized beds in 4.5, 7 3, 9 1, 10, 15, 20.7 and 29.4 cm dia fluidized bed glass columns.

10. Modelling of bubbling fluidized bed reactors

Davidson and Harnson³ showed that bubble gas stays with bubble, recirculating very much like a smoke ring and only penetrating a small distance into the emulsion. This zone of penetration is called the cloud since it envelops the nsing bubble. Rowe and Partindge¹¹ observed experimentally that each bubble of gas drags a substantial wake of solids up the bed These two developments have established the basis for the development of hydrodynamic models using bubble size as parameter. One-, two-, three- and multi-stage models have been developed for bubbling fluidized bed reactors. Each of these models is applicable to the particular regime(s) of bubbling for first order inteversible catalytic reactions with steady-state operation under isothermal conditions. The proposed one- and two-stage complete mixing models are highly suitable for pilot- and semi-industrial scale fluidized bed reactors while the multi-stage complete mixing model and the two-stage pilog flow model are suitable to all flow rates, if the values of static bed height to bed diameter ratio are sufficiently high.

11. Modelling of slugging fluidized bed reactors

Most of the laboratory- and pilot-plant scale reactors operate under slugging condition at moderate bed heights, both with small and big size particles. In the case of big size particles, the phenomenon of slugging is more pronounced even at low bed height to diameter ratio. Thiel and Potter¹² supposed that each slug is followed by a well mixed wake and a piston flow region. The rising velocity of the isolated slug is always greater than the interstital gas velocity at incipient fluidization and clouds are formed around the slug as in the case of a bubble in bubbling fluidized bed. This forms a strong basis for developing models of slugging fluidized bed reactors. One-, two, three- and four-stage models have been developed for slugging fluidized bed reactors. Cone-, two, three- and four-stage models have been developed for slugging for first order irreversible catalytic reactions with steady-state operation under isothermal conditions. The two-stage complete mixing model and the two-stage plug flow model generally predict somewhat lower conversions on account of the domination of the square-nosed slugging phenomenon, while they predict farily well under round-nosed slugging conditions. The one-stage complete mixing model and the one-stage plug flow model predict well under turbulent round-nosed slugging conditions only.

12. Transient modelling

One-stage complete mixing transient models have been developed for vigorous and turbulent bubbling conditions in laboratory- and pilot-scale fluidized bed reactors and round-nosed slugging condition in pilot-scale fluidized bed reactor. The proposed transient one-stage complete mixing model for bubbling fluidized bed reactors has been tested with the experimental data of seven investigators, covering five catalytic reaction systems. Likewise the proposed transient one-stage complete mixing model for slugging fluidized bed reactors has been tested with the experimental data of three investigators, covering three catalytic reaction systems. The overall predicted values of conversion at the eqo of the transient period from the proposed one-stage transient complete mixing model of bubbling/slugging fluidized bed reactors agree well with the steady-state conversion data of other investigators.

13. Scale-up and design aspects

Based on the (i) detailed hydrodynamic investigation in laboratory- and pilot-scale bubbling and slugging fluidized beds (ii) transient analysis of bubbling and slugging phenomenon in laboratory- and pilot-scale fluidized beds and (iii) detailed study of steady- and transientstate modelling of bubbling and slugging fluidized bed reactors, methods have been proposed for the scale-up and design of fluidized bed reactors. Independent dimensionless parameters governing the hydrodynamics of bubbling and slugging phenomena have been proposed for the scale-up of fluidized bed reactor. The applicability of the proposed correlations to predict various hydrodynamic characteristics of bubbling and slugging fluidized beds and proposed steady-state and transient models is illustrated for the design of pilot- and semi-industrial scale fluidized bed reactors.

14. Concluding remarks

The results of this investigation can be exploited to analyse the data from pilot plant tests and suitably employed for the scale-up and design of fluidized bed reactors **HSc THESES ABSTRACTS**

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Thesis Abstract (Ph.D.)

Modification and refinement of aluminium-silicon alloys by strontium, beryllium and phosphorus by V A. Joy

Research supervisors: S Seshan, K.I. Vasu (Central Electrochemical Research Institute, Karaikudi) and C.G. Krishnadas Nair (Hindustan Aeronautics Ltd., Bangalore). Department: Mechanical Engineering.

1. Introduction

- Notice

Aluminium-stiticon alloys are among the most wildely used non-ferrous materials. These alloys are modified by the addition of small quantities of alkaline elements, most popular among them being

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sodium Sodium has been used as the modifier for AI-Si alloys for quite a number of years not withstanding its fuming tendency, problems of recovery and difficulties involved in the control of residual sodium. These are some of the reasons which prompted the search for alternate modifiers such as strontium, antimony, rare earth metals, etc.

2. Results and discussion

An attempt was made to study the behaviour of strontium-modified aluminium-silicon alloys by undertaking a detailed investigation of a series of aluminium alloys containing silicon varying from 6 to 15%. Additional refining of these alloys was attempted using beryllium in the hypo-eutectic alloys for aerospace applications. The refining of hyper-eutectic alloys was achieved by *P* (which was used to refine the primary silicon) and Sr to modify the eutectic silicon.

The effect of holding time on the degree of modification was studied by analysing the microstructures corresponding to each melt with varying holding times and the resultant mechanical properties achieved both in chill and sand castings. It was seen that strontium losses with holding time showed a specific pattern. A relationship between the resultal Sr content and holding time was obtained and was found to be dependent on the initial addition of Sr. The mechanical properties showed an initial improvement for the first two hours of incubation period, subsequently there was a detenoration of properties with holding time.

Al-7%SE0.3%Mg alloy with low iron content (Fe 0.15%) cast in chill moulds after the additions of Srand Be showed excellent mechanical properties, even superior to a similar A337 alloy. This was brought about because of fine dendrite arm spacing, large number of *β*-silicon counts, lower spect ratio of the silicon cell and lower defect level in the casting.

Thermal analysis was carried out for AI-7% SI-0.3% Mg alloy castings with varying section thokness (to achieve differential cooling rates) in order to study the correlation of combined thermal parameters (such as thermal parameter index and gradient acceleration parameter) with microstructural parameters (DAS and cell count) and mechanical properties. Good relationships between these parameters have been obtained

As an extension to the experiments carried out on cast AI-Si alloys, AI-7%Si-0.3%Mg test castings, after sodium and strontium modifications, were forged to study their suitability for forging Although tensile and impact properties of Sr-modified forgings did not show much mprovement over unmodified and Na-modified alloys, the fatigue properties of Sr-modified forgings were superior to those of both unmodified and Na-modified forgings.

It was also found that unmodified and Na-modified forgings cracked very severely whereas the Sr-modified forgings were crack-free, which explained the improved fatigue strength achieved in Sr-modified forgings

The studies on AI-Si alloys with varying silicon content (6, 10, 12 and 15%) were carried out with due emphasis given to the microstructure of each composition, with different additions of Sr and Be individually and in combination. The microstructures of sand castings as well as chill castings in both as-cast and heat-treated conditions were thoroughly analysed Based on these individual microstructures, the parameters such as volume fraction of eutectic, mean-free distance between β -silicon particles, dendrite-arm spacing, number of β -silicon cell counts, aspect ratio of cells, etc., were evaluated Each of these parameters was correlated with the mechanical properties in the course of this investigation, it was found that those AI-Si alloys to which Sr and Be were added possess the maximum ductility among all the hypo-eutectic and eutectic AI-Si alloys studied.

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Two ultra-high strength hyper-eutectic AI-Si alloys have been developed during the course of this investigation with a basic composition of AI-15%Si-0.3%Mg alloy with (i) 0-1-0.2%P addition and (ii) 0.1-0.2%P+0.1% Sr addition. These alloys were chill-cast and then hear treated as per the prescribed cycle of heat treatment. The ultimate tensile strength and percentage elongation recorded for these alloys showed an all time high of 38- 42kg/mm² and 3-.4% respectively. The hardness of the above mentioned alloys was also superior to most of the AI-Si and AI-Cu alloys (except of A390 alloy) in use. These results have been justified by SEM and TEM studies.

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Thesis Abstract (M.Sc.(Engng))

Application of singularity methods in the exact computation of incompressible potential flow by K Leelavathi Research supervisors: V S Holla and N Rajappa (NAL) Denartment Aerospace Engineering

1. Introduction

Panel methods are extensively used at the present time for the design, analysis and evaluation of aerodynamic configurations, because of their ability to meet three major challenges (i) versatility to handle a wide variety of both conventional and unconventional geometrical shapes, is sufficient accuracy to predict details of flow characteristics, and (iii) acceptable, very accommical computer costs in running and executing computer programs based on different methods

Recent applications to a number of practical, contemporary aerodynamic shapes of interest have, however, revealed that the panel methods do not predict surface pressures adequately accurately when the shapes have thin regions on their surface¹⁻⁵ (e.g. low thickness ratio, thin training edges, moderate to heavy camber, etc.). This is rather unfortunate when it is emphasised that the panel methods do not place, unlike thin-airfoil/thin-wing theories, any restriction on the geometry of the shapes. Some attempts have been made to get around the issue by resorting to (i) higher order panel methods, and (ii) panel methods with singularity mixes. No serious nevestigation seems to have been carried out so far to examine the root cause of the problem and formulate a suitable solution strategy based on such understanding. The present thesis is devoted to this task. Since a three-dimensional investigation is computationally quite expensive, the present study has been restricted to two-dimensional profiles. Also, among the various panel methods available for the study, attention has been focussed on the proneering Hess and Smith source panel base method⁵ to illustrate the approach adopted.

2. The root cause of the problem

The Hess and Smith source panel base method approximates the profile by connected straight ine panels and distributes a source distribution of constant strength on each panel. Since the width of the panel is quite small, these assumptions represent the true state of affairs in an average fashion with reasonable accuracy and do not therefore reflect any weakness in the conceptual foundations of the method. It follows then that the observed inaccurate predictions of surface pressure reported for some profiles should be traceable to the the numerical solution of the equations [A] [σ] = [b] for source strengths. The thesis proceeds accordingly to examine the condition number of the panel influence coefficient matrix [A] for normal induced velocities. It is shown that the condition number of matrix [A] has significantly large values whenever the profiles have thin regions on their surface, and this tends to anhance the growth of round-off errors in computation making calculated pressures unreliable and inaccurate

3. The solution strategy

In classical numerical analysis, it is well-known that the problem of ill-conditioning which arises when one attempts to fit a higher degree least square polynomial to observational data, is

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overcome by reformulating the same problem in terms of orthogonal polynomial fit. This suggests that the equations [A] [a] = [b] for source singularity strengths [a], should be rearranged in some way, together with the unknowns [a]. To identify the best way in which this process can be carried out, the thesis examines the structure and properties of the panel influence coefficient matrix [A] for normal induced velocities. A new theory is formulated for solving the equations [A] [a] = [b]. The matrix equation is first rewritten in the form [C] [a] = [b] - [D][a] where the relative decomposition [A] = [C]+[D] is evolved from the properties of [A] following from the relative geometry of the profile upper and lower surfaces. The equation [C] [a] = [b] - [D][a] is then folded and defolded about the profile chord. It is shown that the resulting coupled systems of linear equations are very well-conditioned and give uniformly reliable and accurate predictions.

4. Discussion

It is to be noted that the new formulation proposed in this thesis has added to the versatility of the



Fig. 1. Extremely thin airfoil section, comparison between NLR (1972) Panel method and exact solution of a flat plate^2



Fig 2 Pressure distribution

Hess and Smith source panel base method very significantly by removing the inadequacies reported earlier in the prediction of surface pressures for profiles with thin regions on their surface

Another point worthy of mention is the very favourable consequences of the new formulation for computationally cost-effective *i.e.* faster solution of the equations for source singularity strengths. The number of iterations for arriving at a converged solution is significantly smaller in the case of the new formulation. Also, the rate of convergence has been observed to be more rapid as the profile decreases in thickness (Table I).

The present work has also shown that, for profiles with concave regions on their surface, the new formulation consistently predicts surface pressures with very good accuracy when used with a 0.3 power law vorticity distribution, despite being based on a low-order method (fig. 2). Since the current approaches for such profiles invariably invoke a higher order method with parabolic vorticity, the new formulation proposed in this thesis appears to be quite attractive and better.

Profile	Hess and Smith	Present	_
VACA 0012	111	56	
2412	117	68	
0001	1197	140	
2401	1542	184*	
JOUK 1200	9371	84*	
1204	1256+	110*	
1220	2049 *	127*	
1318	1739 -	121*	
0100	11322	179*	
0104	15643 '	233*	

Table I Iterations for convergence

* parabolic vorticity law used, *0.3 power vorticity law used

5. Conclusion

The work reported in this thesis represents the first detailed study devoted to the structure of the influence coefficient matrix in a panel method and its favourable consequences for laster convergence to solution for singularity strengths. Extensions of this work based on (i) different types of singularities, (ii) multi-component profiles in two and three dimensions, (iii) higher order panel methods, etc., would undoubtedly pave the way eventually for obtaining surface pressures on any configuration at very low and highly economical computational costs.

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Thesis Abstract (M.Sc (Engng))

Characterisation of rapidly solidified aluminium-iron alloys by C.S. Lakshmi. Research supervisors: R.M. Mallya and E.S. Rajagopal. Department: Metallurgy (Interdisciplinary area — Materials Science).

1. Introduction

Rapid solidification processing is currently of great interest in offering potentially superior materials for high performance applications. In recent days developments in aerospace and automobile industries and materials based on aluminium with high mechanical strength as well as thermal stabilities spurring considerable research work on the development of rapidly solidified aluminium-based alloys Among the various aluminium-based alloys subjected to RSP, the aluminium-iron system has been extensively studied because of its high-temperature applications.

Recently the observation of icosahedral rotational symmetry in several alloy systems like Al-Mn¹ has raised considerable interest in materials scientists and physicists². Aluminium-iron system is expected to possess such a symmetry over a certain range of composition.

2. Experimental programme

The present work is an attempt to look at the microstructural aspects of rapidly solidified AI-Fe alloys of various compositions. Alloys of five compositions have been chosen and all the samples are characterised by X-ray diffraction and transmission electron microscopic techniques.

The Al-10 wt % Fe alloy strips have been prepared in our laboratory by the twin roller technique, by quenching the alloy from three different quenching temperatures (T_q) namely 920, 960 and 100°C The Al-3.6 wt % Fe-1 wt % Misch metal alloy strips have been heat-treated at 350°C for three intervals of time, namely, 20, 46 and 66 h.

In Al-Fe alloys with compositions Al-26.20 wt % Fe (14 at % Fe), Al-32.38 wt % Fe (18 at % Fe) and Al-42.10 wt % Fe (25 at % Fe) (all prepared by melt spinning technique at DMRL, Hyderabad), the quasicrystalline phases showing five-fold electron diffraction patterns have been investigated.

In all the above mentioned alloys X-ray diffraction and transmission electron microscopy techniques have been extensively used to characterise the structures. The strip specimens having electron transparency have been prepared using the jet technique, the electrolyte maintained at -30° C

3. Results and conclusions

The microstructures of AI-10 wt % Fe alloy quenched from different temperatures (T_q) are similar to those reported by Jones³ and Jacobs *et al*⁴. Electron micrographs show two distinct zones, A

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and B In addition, the samples quenched from 960 and 1000°C show needle structures. Lattice parameter measurements by X-ray diffraction data indicate a decrease in lattice parameter with an increase in temperature of quenching. According to Jacobs *et al* the crystallites of zone A in AI-8 wt % Fe are of simple cubic structure with lattice parameter *a* = 360 Å. But the ring patterns obtained in the present TEM studies indicate their structure to be face-centred cubic with a = 347 Å ($T_q = 960^{\circ}$ C) and a = 353 Å ($T_q = 1000^{\circ}$ C)

The microstructural aspects of AI-3.6 wt % Fe-Misch metal is also investigated X-ray studies show a slight increase in the lattice parameter on heat treatment. The as-quenched as well as the heat-treated strips of this alloy have a microhardness of 85 kg/rmn²² and TEM studies and microhardness measurements are indicative of their thermal stability⁵.



F s 1 Electron diffraction patterns corresponding to (a) 5-fold symmetry, (b) [710] direction, (c) $[\bar{1}r^{2}0]$ direction, (d) T-phases

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In alloys with composition of Al₈₆Fe₁₄, Al₈₂Fe₁₈ and Al₇₅Fe₂₅ quasicrystalline phases showing five-fold symmetric electron diffraction spots have been observed. Two-and three-fold axes are found at angles of 58.3 and 37.4° respectively with respect to five-fold axes, in accordance with the toosahedral symmetry considerations. An additional pattern corresponding to [710] direction⁶ has been observed in Al₈₆Fe₁₄ and Al₈₂Fe₁₈. A fifth diffraction pattern corresponding to [$\overline{17}^{20}$] has been observed in Al₈₆Fe₁₄ and the ternary system Al-18 at % Mn-1 at % Fe. Some electron diffraction patterns are shown (fig. 1)

The quasilattice constant has been calculated to be 4.57 Å for Al₇₅Fe₂₅ alloy. The T-phases⁷ have also been found to be present in Al₇₅Fe₂₆ alloy. While the twinning model has been hypothesised by Pauling⁶ and others⁹, the results are briefly discussed in the light of the existing theories of quasicrystals from the point of view of Penrose¹⁰ type of tiling.

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